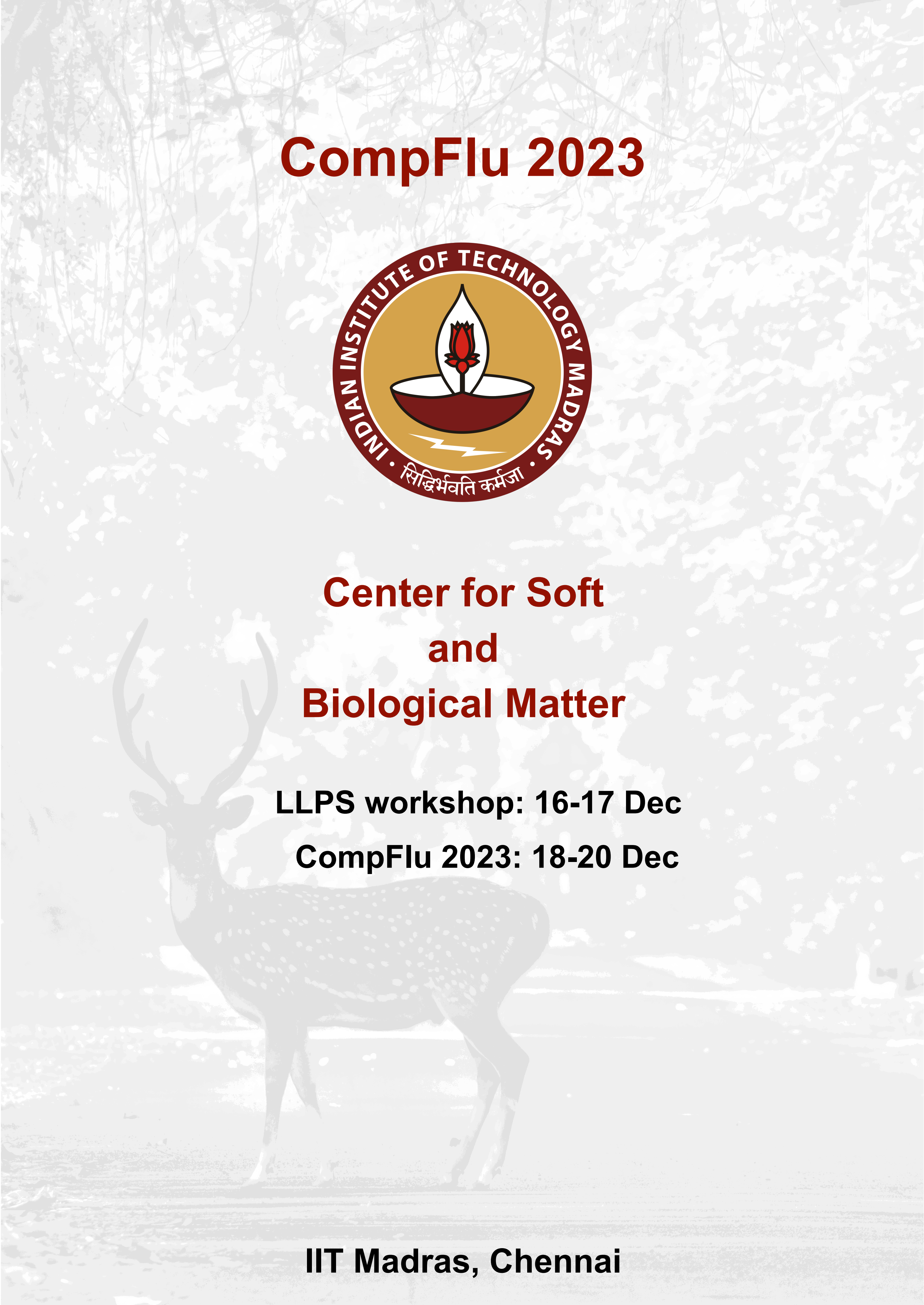

CompFlu 2023

Center for Soft and Biological Matter

LLPS workshop: 16-17 Dec
CompFlu 2023: 18-20 Dec

IIT Madras, Chennai

ACTIVE MATTER

ORAL PRESENTATION

ACTIVE MATTER SESSION 1 - 19-12-2023

Time	Speaker	Title	Abstract ID
9:00 AM	Snigdha Thakur	Collapse Dynamics of Flexible Active Polymer	AM - O10
9:30 AM	Nitin Kumar	Active Matter with Robots	AM - O2
10:00 AM	Bibhu Ranjan Sarangi	An active particle at a soft interface	AM - O7
11:00 AM	Soumik Das	Bioinspired Soft Matter Using Solitons in Liquid Crystals	AM - O3
11:30 AM	Arnab Saha	Microscopic Gyration with Dissipative Coupling	AM - O5
12:00 PM	Vijayakumar Chikkadi	Phase seperation of passive particles in active liquids	AM - O6

ACTIVE MATTER SESSION 2 - 20-12-2023

8:30 AM	Akash Choudhary	How viscoelasticity influences the orbital dynamics, microstructure and rheology of dilute active suspensions	AM - P18
9:00 AM	Harinadha Gidituri	Swimming Efficiently by Wrapping	AM - O4
9:30 AM	Sunil Pratap Singh	Characteristic features of self-avoiding active polymers under shear flow	AM - P19
10:30 AM	H R Vutukuri	Sculpting vesicles with active particles: Less is more	AM - P47
11:00 AM	Debasish Chaudhuri	How do activity and inertia control non-equilibrium features of active Brownian particles?	AM - P46
11:30 AM	Rajesh Ganapathy	TBD	

ACTIVE MATTER SESSION 3 - 20-12-2023

2:00 PM	Jason Picardo	How turnover triggers nonlinear waves in the active actomyosin cortex	AM - P40
2:30 PM	Tapan C. Adhyapak	Controlled dynamics of microbes in confinements: how to exploit shape and flexibility	AM - P38
3:00 PM	Arvin Subramaniam	Emergent rigidity in chemically self-interacting active polymers	AM - P6
4:00 PM	Sayan Das	Spontaneous motion of isotropic particles in a Carreau fluid	AM - P1
4:30 PM	Dileep Mampallil	Dynamics of Nucleating Microdroplets at the Contact Line of Evaporating Multicomponent Drops	AM - P13
5:00 PM	Suchismita Das	Flocking by turning away	AM - P48

POSTER PRESENTATION - 18-12-2023

Sl. No	Speaker	Title	Abstract ID
1	Biswajit Das	Collapse Dynamics of Flexible Active Polymer	AM - P2
2	Simran Kapoor	Active Particle Suspensions In Viscoelastic Fluids	AM - P3
3	Rishish Mishra	Interfacial Pusher Bacterium	AM - P4
4	Surabhi Jaiswal	Particle-based mesoscopic model for phase separation in a binary fluid	AM - P5
5	Alakesh Upadhyaya	Stochastic migration dynamics of Marangoni surfers between two chambers	AM - P7
6	Sandeep Kumar	Local Polar and Long-Range Isotropic Activity Assisted Swelling and Collapse Dynamics of an Active Ring Polymer	AM - P8
7	Chandranshu Tiwari	Collective Dynamics of Active Janus Colloids Using Computer Simulations	AM - P9
8	Pawan Kumar	Active droplets dynamics and collective behavior in a capillary	AM - P10
9	Shubhadeep Mandal1	Active Droplets in Gravity	AM - P11

10	Arindam Panda	Characteristic features of self-avoiding active Brownian polymers under linear shear flow	AM - P12
11	Suvendu Kumar Panda	Light-activated rod-shaped colloidal microswimmers for exhibiting multimode dynamics	AM - P14
12	Megha.Varma	Self-propulsion behaviour of cubic shape Janus particles: Effect of shape anisotropy on longer range ballistic motion	AM - P15
13	Siji S. Saju	Tumbling dynamics of an active filament in simple shear flow	AM - P16
14	Srikanta Debata	Self-propelled microrobot for pH sensing applications	AM - P17
15	Sumant Pandey	Nematic Droplets in Structured Optical Field	AM - P20
16	Pradeep Kumar Yadav	Effect of real-space circulating currents on the bubble phase separation of active particles	AM - P21
17	Abhishek Sharma	Phase Transition In Active Nematics	AM - P22
18	Ann Rosna George	RODROLLS: Self Rolling Rods powered by Light and Chemical gradients	AM - P23
19	Harishwar Raman	Pair and Collective Dynamics of Active SiO2-Pt Active Janus Colloids	AM - P24
20	Dhananjay Gautam	Enhanced Activity Reduces the Duration of Intermittent Lévy Walks in Bacterial Turbulence	AM - P25
21	Hemlata Meena	Universal scaling underlying the evolution of bacterial interfaces: A case study on swimmers vs. non-swimmers	AM - P26
22	Uttam Kumar	Dynamics of Bacterial Swarming on a Solid Porous Media	AM - P27
23	Smita S. Sontakke	Soft makes it hard to swim: Role of microconfinement elasticity in active swimmer dynamics	AM - P29
24	Shreyas A. Shenoy	Dynamics of an active Belousov-Zhabotinsky droplet in shear flow	AM - P31
25	Baburao Simma	Dynamics of the asymmetrical self propelled particle in a ordered crowded environment	AM - P32

26	Biswajit Maji	Coarsening arrest by active-rotor turbulence in a binary-fluid system	AM - P33
27	Devi Prasad Panigrahi	Motility Induced Phase Separation in Quorum Sensing Particles	AM - P34
28	Shubhendu Shekhar Khali	When does an active bath behave as an equilibrium one?	AM - P35
29	Jaideep Vaidya	Spontaneous flow transition of active nematics in a wavy walled channel	AM - P36
30	Byjesh Nalini Radhakrishnan	Measuring entropy production in active turbulence	AM - P37
31	Sanatan Halder	Ergodicity breaking in harmonically bound active dynamics	AM - P39
32	Arjun S R	A Study on the Transport Properties of Active Brownian Particles in Asymmetric Ratchet Potential	AM - P41
33	Mayurakshi Deb	Colloidal transport by active dimers	AM - P42
34	Ambareesh Shrivastav	Hydrodynamics of flagellated microswimmers in confined fluids	AM - P44
35	Thilak Raj	Unveiling the propulsion dynamics of active patchy colloids using optical tweezers	AM - P45

BIOLOGICAL MATTER

ORAL PRESENTATION

BIOLOGICAL MATTER SESSION 1 - 18-12-2023

Time	Speaker	Title	Abstract ID
9:00 AM	Madan Rao	The effervescent cell membrane: nonequilibrium driving and active emulsions	BM-O12
9:30 AM	Soudamini Sahoo	Influence of non-equilibrium switching of segmental states on chromatin compaction	BM - O1
10:00 AM	Ranjith Padinhateeri	Computing polymer properties of chromatin from contact map data	BM-O8
11:00 AM	Shivprasad Patil	Viscoelasticity of single-folded protein using dynamic atomic force microscopy	BM-O4
11:30 AM	Mahipal Ganji	Biophysical approaches to understand genome organization	BM-O9
12:00 PM	Deepak Bhat	Speed variation of bacterial replisomes	BM-O2

BIOLOGICAL MATTER SESSION 2 - 18-12-2023

Time	Speaker	Title	Abstract ID
2:30 PM	Tapomoy Bhattacharjee	Single-cell morphology dictates bacterial population growth under 3D confinement	BM-O13
3:00 PM	Tripta Bhatia	Lipid Vesicles Adhesion mediated by Sugar-Cleaving Enzyme Invertase	BM-O3
3:30 PM	Srividhya Parthasarathi	Antibiotic-Induced Bacterial Membrane Dynamic Alterations unraveled by Super-Resolution Nanoscopy	BM-O10
3:45 PM	Sandeep K. Rai	Elucidating the Multifaceted Nature of Multiphasic Condensates in Neuronal Diseases	BM-O11
4:30 PM	Philip Pearce	Pattern formation by living droplets in chemoattractant gradients	BM-O5

5:00 PM	Ushashi Roy	Emergent spatiotemporal multistability enabled by the bio-mechanical underpinnings of different gene regulatory network motifs	BM-O6
5:30 PM	Ramya Koduvayur	The hieararchical structure and complex rheology of mucins	BM-O15
5:45 PM	Abhilasha Batra	Decoding of temperature signals by the thermosensory neurons in Caenorhabditis elegans	BM-O14

POSTER PRESENTATION - 20-12-2023

Sl. No	**Speaker**	**Title**	**Abstract ID**
1	Chaithanya KVS	Homeostasis in confined environments	BM - P1
2	Ashitha B A	Yeast Budding Dynamics in Complex 3D Environments	BM - P2
3	Sreepadmanabh M	Cellular growth and behavior in designer 3D culture media	BM - P3
4	Jorge R. Espinosa	Location and Concentration of Aromatic-Rich Segments Dictates the Percolating Inter-Molecular Network and Viscoelastic Properties of Ageing Condensates	BM - P4
5	Ashok Kumar Dasmahapatra	Disruption of Alzheimer’s Amyloid-β Fibrils: Insight from all-atom Molecular Dynamics Simulation Study	BM - P5
6	Nandhu Krishna Babu	Role Of Tissue Mechanics In Wound Healing In An Epithelial Monolayer	BM - P6
7	Shreerang Pande	Topology-driven spatial organization of ring polymers under confinement	BM - P7
8	Garima Rani	Entropic insights on emerging traits from growing bacterial colonies	BM - P8
9	Bincy Lukose	Homo- versus Hetero-Oligomerization Drives the Thermo-Osmo Responsive Behavior of the Enterobacterial Sensory Protein H-NS	BM - P9

10	Sanchari Chakraborty	Understanding Phase Separation Characteristics of Non-Amyloid β-Component of α-Synuclein	BM - P11
11	Saloni Goyal	Conformation and Charge - Density Dependent Phase Separation and Ageing of an Intrinsically Disordered Protein	BM - P12
12	Anirban Paul	Molecular dynamics investigation of the dynamical response of the interfacial waters near DPPC bilayer to Hyaluronic acid	BM - P13
13	Sweta Pradhan	Protein Association Reaction Study on GB1 Protein Dimerization in a Crowded Environment	BM - P14
14	Sahithya Sridharan Iyer	Role of WASP in Arp2/3 complex activation	BM - P15
15	Anagha Manohar	pH mediated aggregation and fibrillization of amyloid beta(16-22)	BM - P17
16	Rajendra Rath	Association of Globular and Intrinsically Disordered Proteins in Particle Based Coarse-grained Models	BM - P18
17	Ashish Joshi	Single-droplet single-molecule FRET and vibrational Raman scattering reveal conformational heterogeneity and shapeshifting within liquid condensates	BM - P19
18	Lisha Arora	Complex coacervation of a prion-like protein and a J-domain protein into multiphasic condensates inhibits the amyloid formation	BM - P20
19	Deepshikha Ghosh	Investigating the Chaperone Mechanism of α-Crystallin in Preventing γDCrystallin Aggregation in Cataract Formation	BM - P21
20	Deepshikha Ghosh	Exploring the molecular aspects of α-crystallin's inhibitory role against γD-crystallin aggregation	BM - P22
21	Anushka Biswas	Predictive Modeling of Biological Enzyme-Substrate Binding: Understanding Conformational Dynamics and External Influences	BM - P23

22	Ajoy Paul	Liquid-liquid phase separation of p53 and its paralogs p63 & p73 in the context of cancer progression.	BM - P25
23	Monika Choudhary	Multicomponent membranes with active recycling: compositional inhomogeneities and morphology	BM - P26
24	Anurag Singh	Amylin modulates the electrical properties of Amyloid-β during its fibril growth	BM - P27
25	Akshay Narayan Sarangi	Impedance spectroscopy revealed the surfactant-driven unfolding and refolding of a globular protein.	BM - P28
26	Harini SureshKumar	Signatures of glassy dynamics in liquid-ordered lipid membrane	BM - P30
27	Mahrukh A Mir	Smearing Technique For Liquid Viscosity Measurement	BM - P31
28	Uttam Kumar	Dynamics of Bacterial Biofilm Growth on Porous Surfaces: Insights from a Three-Phase Model	BM - P32
29	Shovon Swarnakar	Nanoscale Dynamic Interplay of SARS CoV Fusion Peptides and Lipids in Host Cell Entry	BM - P33
30	Nehal Mathur	Pulling Short DNA with Mismatch Base Pairs	BM - P34
31	Rupal Kaushik	Synthesis of highly biocompatible surface-modified MoS2 Nanoflowers: unraveling the detailed antibacterial mechanisms	BM - P35
32	Prabhash Kumar	Understanding the role of convective mixing on aerosols deposition in lung acini	BM - P36
33	Omkar S. Deshmukh	Understanding Mucin-Albumin assembly using microrheology	BM - P37
34	Sandeep Parma	PNIPAAm as A Thermosensitive Drug Delivery System for Targeted Cancer Treatment: A Molecular Dynamics Study	BM - P38
35	Bratin Kumar Das	Probing the formation of pre-fibrillar prion peptide oligomer with atomistic molecular dynamics simulation	BM - P39

36	Sesan Nayak	Super-hydrophobic surface assisted micro-droplet drying for aerosol evaporation analysis	BM - P40
37	Semanti Mukherjee	Role of Liquid-liquid Phase Separation in the Regulated Secretory Pathway	BM - P41
38	Sumangal Roychowdhury	Conformational fluctuation can modulate the phase separation of yeast prion protein	BM - P42
39	Tanmoy Pal	Phase Separation of Intrinsically Disordered Proteins in Analytical and Field Theoretic Models	BM - P44
40	Bhukya Vijay Mohan	Force measurements on cells and Near-field optical microscope platform	BM - P45
41	Puchalapalli Saveri	Rheological characterization of bacterial suspensions in plant mucilage	BM - P46
42	Debalina Datta	Phase separation of p53 and its functional implications	BM - P47
43	Anirban Paul	Molecular dynamics investigation of the dynamical response of the interfacial waters near DPPC bilayer to Hyaluronic acid	BM - P48
44	Moumita Sasmal	Biomimicking Of The Natural Mucilage By Pectin-based System	BM - P49
45	Shouvik Manna	Mechanism of nucleation and liquid-to-solid transition for α-synuclein liquid-liquid phase separation	BM - P50

COLLOIDS

ORAL PRESENTATION

COLLOIDS SESSION 1 - 18-12-2023

Time	Speaker	Title	Abstract ID
9:00 AM	Eric Grelet	Decorating Filamentous Viruses: Design & Self-Organization of Virus based Colloidal Molecules	CO-P45
9:30 AM	Sulalit Bandyopadhyay	Coating Hydrophilic and Hydrophobic Iron Oxide Nanoparticles with Polymers using Novel Flash Nanoprecipitation Techniques.	CO-O2
10:00 AM	Manisha Jhajhria	Activity induced non-monotonic aggregation in a mixture of chemically active and passive particles	CO-O1
10:15 AM	Om Prakash Bamboriya	Critical cracking thickness of mixed particles suspension film	CO-P23
11:00 AM	Subramanyan Namboodiri Varanakkottu	Light-controlled patterning of metallic nanoparticles	CO-O7
11:30 AM	Ashish Kumar Thokchom	Bioinspired structures via self-assembled of colloidal particles	CO-O3
12:00 AM	Ashutosh Shukla	Opto-thermoelectric trapping of fluorescent nanodiamonds	CO-O4
12:15 AM	Sonali Kawale	Slow dynamics of a soft glassy colloidal suspension in the presence of probe particles	CO-P38

COLLOIDS SESSION 2 - 19-12-2023

9:00 AM	Rahul Mangal	Pe dependent pair interactions in self-propelled droplets	CO-O5
9:30 AM	Prashant Kumar	Hybrid Metamaterials with Controllable Twist	CO-06
10:00 AM	Mamta Yadav	Effective one-component theory for colloidal suspensions	CO-P24
10:15 AM	Soumyajyoti Chatterjee	Particle-Stabilized Microcapsules via Ice Templating	
11:00 AM	H S S Ramakrishna Matte	Solution Processing of Low-dimensional Materials and Applications	CO-O8
11:30 AM	Pramod P. Pillai	The Impact of Surface Ligands in Regulating Nanoparticle Chemistry	CO-P46
12:00 AM	Jyoti R. Seth	Engineering Polymers and Colloidal Particles to Control and Tailor Crystal Habit	CO-P47

POSTER PRESENTATION - 19-12-2023

Sl. No	Speaker	Title	Abstract ID
1	Syamjith KS	Role of Softness on transition temperatures for PNIPAM Microgels	CO-P1
2	Aakriti Sharma	Bulk nanobubble generation by gas supersaturation method	CO-P4
3	Barros Indira	Electric Field Induced Self Assembly of Polystyrene Spheres	CO-P7
4	Sayanth RC	Field Induced Self Assembly of Anisotropic Particles	CO-P8

5	Hariharan Sekar	Development of Antibacterial Waterborne Polymeric Coatings using Iodine Complex	CO-P9
6	Goga Ram	Understanding the effect of Methyl group of molecules in polymer solutions	CO-P10
7	Noman Hanif Barbhuiya	Direction-dependent Dynamics of Colloidal Particle Pairs and the Stokes-Einstein Relation in Quasi-Two-Dimensional Fluids	CO-P12
8	Debasish Saha	Work distribution of a colloid in an elongational flow field and under Ornstein-Uhlenbeck noise	CO-P13
9	Rahul Chand	Optothermal Chiral Rotation in a Trap	CO-P19
10	Chaudhary Eksha Rani	Optical and Optothermal forces on Colloids in Evanescently generated Plasmofluidic Field	CO-P20
11	Lokesh Soni	Electrostatic self-assembly of GO-CNT nano-hybrid structures	CO-P21
12	Meenakshi	Long Range Electrostatic Screening in Zwitterionic Liquids	CO-P22
13	Aditi Dahake	Synthesis of monodispersed Polyethylene nanoparticles by microemulsion	CO-P25
14	Salini Kar	Monitoring the MOF synthesis and quality using sessile drop drying phenomena	CO-P26
15	Farida Batool	Phase Separation in Binary Strongly Coupled Plasma	CO-P27
16	Rajeev Reddy Sadu	Dynamics Of Particles In Line Plumes	CO-P29

17	Neethu Thomas	Tailoring the dimensions of silver nanowires (Ag NW) by modifying the polyol synthesis and the fabrication of Ag NW-based transparent conducting films	CO-P30
18	Santhra Krishnan P	All-natural Plant-derived Superhydrophobic Wax Coatings	CO-P33
19	Chetteente Meethal Ragisha	Plasmonically controlled patterning of metallic nanoparticles at liquid- liquid interface	CO-P34
20	Sanjib Majumder	Pattern formation in microgel laden sessile droplets: Effect of substrate temperature	CO-P35
21	Sk Jasim	Coffee stain morphologies obtained by drying suspension droplets of gold nanorods of different aspect ratios	CO-P36
22	Ejaz Ashraf	Non-linear fluctuating hydrodynamics of a colloid near a plane surface	CO-P37
23	Sankar Hariharan	Quantitative Characterization of Deposit Patterns Formed from Dried Dispersion Drops	CO-P39
24	Simmie Jaglan	Reversibly Aggregating Binary Colloidal System	CO-P40
25	Prathyusha S Nair	Enhancement in the transport properties of a tilted rough ratchet	CO-P42
26	Ramana Patibandla	Sphere motion in a viscous, stratified fluid	CO-P44
27	Santosh Vasant Daware	Synthesis and Characterization of 2D Colloidal Sheets	CO-P48

EARLY CAREER RESEARCHERS

ORAL PRESENTATION

EARLY CAREER RESEARCHERS - 19-12-2023

Time	Speaker	Title	Abstract ID
02:30 PM	Rishabh V More	Micromechanics of particulate soft matter: the governing role of interparticle interactions	EC-O3
03:00 PM	Swati Mehta	Unveiling the Self-Pinning Driven Jamming Behavior of Colloids during Droplet Drying	EC-O1
05:30 PM	Akhil Varma	Morphogenesis of active fluid surfaces: a mechano-chemical model	EC-O4
06:00 PM	Shibananda Das	Sequence-specific folding of active macromolecules	EC-O5
06:30 PM	Praneet Prakash	Spatio-temporal dynamics of nutrient exchanges	EC-O6

POSTER PRESENTATION - 19-12-2023

Sl. No	Speaker	Title	Abstract ID
1	Kandalam Ravitheja	Role of Contact Inhibition of Locomotion in collective behavior and de-mixing of cell types	EC - P1
2	Dipanjan Mandal	Nucleation in the presence of static/dynamic impurities with varying interaction strength in an Ising lattice-gas model of solute precipitation	EC - P2
3	Afroz Momin	A Computational Study on the Smooth-Wall, Radial Gravity Phenomenon in Granular Flow Through a Wedge-Shaped Hopper	EC - P3
4	Sunil Kumar	Effect of Coarse Particle Shape on Mixing and Segregation Dynamics: Insights from Experimental and Discrete Element Method Analyses	EC - P4

5	Pawan K Pandey	Drug Delivery from Ocular Implant: An In-silico Investigation	EC - P5
6	Divya Jayoti	Functionally graded shape reprogrammable liquid crystal elastomers films for artificial gripper applications	EC - P6

EMULSIONS AND FOAMS

ORAL PRESENTATION

EMULSIONS AND FOAMS - 18-12-2023

Time	Speaker	Title	Abstract ID
2:30 PM	Emmanouil Chatzigiannikis	The effect of interfacial stresses on film drainage	EF-O2
3:00 PM	John Crocker	TBD	EF-O3
3:30 PM	Soumodeep Biswas	Light-induced destabilization of oil-in-water emulsions using light-active Bolaform surfactants	EF-P7
4:30 PM	Venkateshwar Dugyala	Novel way to design Pickering emulsions with partial droplet coverage	EF-O1
5:00 PM	Chandra Shekhar	A simple pathway to fabricate water-in-water emulsion-filled gels	EF-O5
5:30 PM	Hemant Kumar	Controlled Phase Inversion of Pickering Emulsions via Particle Surface Engineering	EF-P6
5:45 PM	TBD		

POSTER PRESENTATION - 18-12-2023

Sl. No	Speaker	Title	Abstract ID
1	Rahul Painuly	Drop Interfaces Interaction Under Application of Electric Field: Effects of Surfactants and Polymer	EF-P1
2	Madhavi Tiwari	Preparation of Pickering Double Emulsions by In-situ Particle Surface Modification	EF-P3
3	Senthan Pugalneelam Parameswaran	Evaporative Phase Separation in Polymer Micro-droplets with Confinement and Internal Flow	EF-P4
4	Guguloth Naresh	Numerical Simulations of Instability in Pickering Emulsions Caused by a Mutually Soluble Solute	EF-P5

5	Anjali Kumari	Breaking the Mold: A Novel Approach to Evolving Drop Breakup Functions and Rates Based on Multi-Physics Mechanisms in High Shear Mixers	EF-P8
6	Roopesh P	Oil in water Emulsion Stabilized by HEUR Polymers	EF-P9

FOOD SCIENCE

ORAL PRESENTATION

FOOD SCIENCE - 20-12-2023

Time	Speaker	Title	Abstract ID
8:30 AM	P. Prabhasankar	Application of Empirical and Fundamental Rheology to understand the wheat flour and non-wheat flour Dough properties and its relationship with end products	FS-O1
9:00 AM	Trivikram Reddy	Food science – A soft matter perspective	FS-O2
9:30 AM	Gurmeet Singh	Application of twin-screw extruder for protein texturization: Interplay of system & process parameters on product properties	FS-O3
10:30 AM	Rekha S. Singhal	Emerging trends on formulations of bigels, their rheological characterization and correlation to food applications	FS-O4
11:00 AM	KSMS Raghavarao	Recent Research Developments & Future directions in Food Processing	FS-O5
11:30 AM	Chirasmita Panigrahi	Rheological study of cereal based fermented food suspensions	FS-O6

POSTER PRESENTATION - 18-12-2023

Sl. No	Speaker	Title	Abstract ID
1	Somnath Basak	Rheological characterization of composite hydrogels fabricated from pea protein and konjac glucomannan	FS-P1
2	M. Saravanan	A bottom-up understanding of the rheological and microstructural characteristics of edible oleogels	FS-P2

3	Sree Nivetha. B. B	Formation and characterization of polysaccharide-based oleogel derived from emulsion: A Rheological Investigation	FS-P3
4	Jayaraman K	Study on Evaporation of Liquid Sugarcane Juice Droplet for Granular Jagerry Production	FS-P4
5	Abdul Mateen	Unveiling Rheological Transformations in High Moisture Extrusion: Bridging Insights from Raw Material to Extruded Meat Analogues	FS-P5
6	Manoj Mathpati	Low Moisture Extrusion for Textured Vegetable Protein (TVP) Production from Soy and Pea Protein Isolates: System Response, Expansion Ratio and Rehydration Properties	FS-P6

GELS AND GLASSES

ORAL PRESENTATION

GELS AND GLASSES SESSION 1 - 18-12-2023

Time	Speaker	Title	Abstract ID
9:00 AM	Srikanth Sastry	Low temperature dynamics in a model glass former	GG - O7
9:30 AM	Murali Krishnan	Fatigue Damage of Bituminous Binders using Large Amplitude Oscillatory Shear	GG - O12
10:00 AM	Mounika Gosika	On the structure-viscoelasticity relationship of reversible polymer networks	GG - O8
11:00 AM	Smarajit Karmakar	Dramatic growth of Dynamic and Static correlations in Active Glass-forming Liquids as probed via rod-like probe particles	GG - O9
11:30 AM	Ankit Singh	Dynamics and structural ordering in binary colloidal-solvent mixtures of glass-formers	GG - O3
12:00 PM	Sayantan Majumdar	Inter-particle adhesion induced strong mechanical memory in a dense granular suspension	GG - O2

GELS AND GLASSES SESSION 2 - 19-12-2023

9:00 AM	Yogesh Joshi	A Curious Case of the Thixotropic Timescale	GG - O1
9:30 AM	Harish Srinivasan	Nature of universal subdiffusion crossover in molecular glass-formers	GG - O13
10:00 AM	Santosh Mogurampelly	Ion diffusion, ion-pair relaxations and viscosity of pectin-[BMIM][PF6] electrolytes	GG - O6
11:00 AM	Dimitris Vlassopoulos	Rheology modification with polymeric loops	GG - O14
11:30 AM	Bhaskar Sen Gupta	Dynamics of supercooled liquid in complex confined geometry	GG - O5

12:00 PM	Prachi Thareja	Applications of κ-carrageenan hydrogels strengthened by mixed salt for 3D printing and water remediation	GG - O11

POSTER PRESENTATION - 18-12-2023

Sl. No	Speaker	Title	Abstract ID
1	Saumya Suvarna	Transport properties of a fluid intercating via Mie potential	GG - P1
2	Meenakshi L	Characteristics and correlations of nonaffine particle displacements in the plastic deformation of athermal amorphous materials	GG - P2
3	Hema Teherpuria	Effects of Salt Concentration on EC-LiTFSI Electrolytes	GG - P3
4	Sipra Mohapatra	Ion Transport Mechanisms in PEO-SN-LiTFSI Electrolytes	GG - P4
5	Hitesh Yadav	Molecular dynamics simulations of the effect of fluorinated ethylene carbonate on sodium ion battery electrolytes	GG - P5
6	Sruthi H	New Approach to Prepare FmKP based Supramolecular Organo-Gels	GG - P7

GRANULAR MATERIALS

ORAL PRESENTATION

GRANULAR MATERIALS SESSION 1 - 18-12-2023

Time	Speaker	Title	Abstract ID
2:30 PM	Shankar Ghosh	Self-organization of granular systems under chiral driving	GM - O8
3:00 PM	Tejas Murthy	Mechanical behaviour of cohesive frictional granular materials	GM - O6
3:30 PM	Alok Tiwari	Determination of rotational coefficient of restitution from DEM simulation of vibro-fluidized particles	GM - O4
3:45 PM	Manish Mandal	Novel energy dissipation mechanism in granular mateials under high speed impact	GM - O5
4:30 PM	V Kumaran	Steady and oscillatory states in the granular flow through a vertical channel	GM - O1
5:00 PM	Anurag Tripathi	Role of elasticity and cohesion for accurate and efficient simulations of cohesive granular materials	GM - P17
5:30 PM	Sukhada Bhure	Spherical tracer induced clogging behavior of aspherical particles in a silo	GM - O2
5:45 PM	Sujith Reddy Jaggannagari	A numerical study for multi-layer powder spreading in metal additive manufacturing	GM - O3

POSTER PRESENTATION - 20-12-2023

Sl. No	Speaker	Title	Abstract ID
1	Tarun De	Flow kinematics and stress comparison of resolved and multi-level coarse-grained DEM simulations	GM - P1
2	Vighnesh Prasad	Influence of rheology on the pipeline transportation of mineral slurries	GM - P2

3	Kiran Kumari	Assessment of Segregation for Non-spherical Cohesive Particles using DEM	GM - P3
4	Deepak Pawar	Granular Morphology Matters: Deformation Mechanics of Lithium-Based Pebbles under Triaxial Compression	GM - P4
5	Ravindra Ghodake	Flow behavior of lubricated granular media across various flow configurations	GM - P5
6	Md Shahid Ansari	Flow characterization of poly-dispersed granules under the influence of external mechanical vibration for additive manufacturing applications	GM - P6
7	Afroz Momin	A Computational Study on the Smooth-Wall, Radial Gravity Phenomenon in Granular Flow Through a Wedge-Shaped Hopper	GM - P7
8	Sri Mourya Melam	Two-phase approach for laminar shearing beds using kinetic theory of granular flows	GM - P8
9	Neiladri Sekhar Ray	Kinematics of Granular Surface Flow on a Heap	GM - P9
10	Sarwar Zaheer	Large Scale Industrial Hopper Flow Simulation using coarse-grained DEM	GM - P10
11	Soniya Kumawat	Theory for combined effect of size and density segregation of binary granular mixtures	GM - P11
12	Suchintika Chanda	Continuum modeling of granular flow evolution using OpenFOAM	GM - P12
13	Sourav Ganguli	Turbulence modification of particle-laden flow in horizontal rectangular duct	GM - P13
14	Alok Tiwari	DEM analysis of inelastic rough spherical particles in a vibro-fluidised	GM - P14
15	Mohd Ilyas Bhat	2D DEM study of force transmission during in-plane cutting of flexible granular chains	GM - P15
16	Sanyogita	Dynamics of sand pile	GM - P16

INDUSTRIAL APPLICATIONS

ORAL PRESENTATION

INDUSTRIAL APPLICATIONS - 20-12-2023

Time	Speaker	Title	Abstract ID
8:30 AM	Saswati Pujari	Impact of surfactant chain length and micellization on antimicrobial activity of soap	IA-O1
9:00 AM	Kiran Iyer	Rapid Development of Nirmatrelvir Tablets using Digital Design and Predictive Science	IA-O2
9:30 AM	Anwesha Mohanty	Experimental investigations to study the drug release from bilayer osmotic tablets	IA-O3
9:45 AM	Ashok Yacham	Role of organic ligands on the gas adsorption and separation in Zeolitic Imidazolate Frameworks	IA-O4
10:30 AM	Girish Rao	Shell Bitumen: Innovating from the Refinery to the Road	IA-O5
11:00 AM	Dhiraj Kumar	Application of Analytical Solution of Free Radical Polymerization With AK Method For Semi-Batch Operations	IA-O6
11:45 PM	Rakesh Gupta	Leveraging Bio Digital-Twins for Design and Testing of Formulations and Devices	IA-O7

POSTER PRESENTATION - 18-12-2023

Sl. No	Speaker	Title	Abstract ID
1	Priya Koundle	Effective degradation of dark green rit dye using ozone nanobubbles	IA-P1
2	Bhawana Singh	Predicting Drug Release in Bilayer Osmotic Tablets: Model Development and Experimental Validation	IA-P2
3	Anomitra Saha	Acoustophoresis assisted Fluid Jet Polishing	IA - P5
4	Binu Varghese	Nanobubble modulated Amino acid Adsoprtion at Graphene Surface	IA-P8

MULTIPHASE FLOWS

ORAL PRESENTATION

MULTIPHASE FLOWS - 20-12-2023

Time	Speaker	Title	Abstract ID
8:30 AM	S. Balachandar	Physics-Inspired Machine Learning for Multiphase Flow	MF-05
9:00 AM	Shauvik De	Complex flow behaviors of complex fluids in porous medium for applications in Energy industry	MF-06
9:30 AM	Venkat Gundabala	Microfluidics Route to Generation of Biomaterials	MF-03
10:30 AM	Ganesh Subramanian	An altered streamline topology allows deformed drops to transport mass faster than spherical ones	MF-01
11:00 AM	Dipankar Bandyopadhyay	Self-organized Microrheology of the Suspended Particles at the Mesoscale	MF-04
11:30 AM	Partha Sarathi Goswami	Dynamics of turbulence suspensions with inertial particles	MF-02

POSTER PRESENTATION - 18-12-2023

Sl. No	Speaker	Title	Abstract ID
1	Pavan Kumar Singeetham	Inertio-elastic orientation dynamics of anisotropic particles in linear shearing flows	MF-P1
2	Sourabh Das	Deterministic lateral displacement for precise microfluidic droplet sorting	MF-P2
3	Abhiram Ramachandran	Droplet Impact on Drone Propellers	MF-P3
4	Krishnaveni Thota	Numerical analysis of the migration of a particle in a symmetric serpentine microchannel in inertial microfluidics	MF-P4

5	Shuvalaxmi Das	Effect of size-disparity on the structure and dynamics of a Lennard-Jones mixture with random interactions between the particles	MF-P5
6	Deekshith I. Poojary	Influence of synthetic inflow perturbations on the dispersion characteristics of particles over a normal flat plate	MF-P6
7	Saini Jatin Rao	Dispersion size measurement in multiphase systems using Depth from Defocus technique	MF-P7
8	Supriya Karmakar	Long- and short-time stability analyses of plane Poiseuille flow in an anisotropic porous channel	MF-P8
9	Anushka Herale	A minimal continuum model of clogging in spatio-temporally varying channels	MF-P9
10	Karthick Raj .S	Modeling droplet decisions in 1D microfluidic networks	MF-P10
11	R.Kumar	Elastohydrodynamics Of Faraday Instability	MF-P11
12	Lopamudra Palodhi	Thermodynamic Effects on Viscous Fingering	MF-P12
13	Harishankar Muppirala	Hydrodynamic stability of gravity waves on a free surface: Effect of curvature	MF-P13
14	A.Subramanian	Nonlinear evolution of a Dewetting bilayer thin film on a soft-gel layer	MF-P14
15	Daniya Davis	Phase separation of binary liquid confined inside uniform pore with wetting effect	MF-P15
16	Garima Singh	Film Dynamics Over a Topographical Surface Using Lattice Boltzmann Method	MF-P16
17	Anu V. S. Nath	Clustering and chaotic motion of inertial particles in an isolated vortex	MF-P17
18	Parameshwaran A	Effect of Vicsek like activity on the Vapour liquid phase separation inside cylindrical nanopore	MF-P18

19	Jagadeesh Korukonda	Enhancement of Chemical Reactions using Droplet-Based Microfluidics: A Study on Contact Modes and Reaction Kinetics	MF-P19
20	Shravya Gundavarapu	Evidence of an inertialess Kapitza instability due to viscosity stratification	MF-P20
21	Lokendra Mohan Sharma	Quantitative measurements of immiscible oil jet	MF-P21
22	Sajal Wankhede	Weakly nonlinear analysis of flow driven morphological instability in porous anodic oxides	MF-P22
23	Anurag Pant	Vorticity generation in miscible, volatile film spreading	MF-P23
24	Rajeev Reddy Sadu	Dynamics Of Particles In Line Plumes	MF-P24
25	Charul Gupta	Determining the flow fields near a moving contact line: comparison between experiments and theory	MF-P25
26	Shubham N. Lanjewar	Behavior of Confined Gas Bubble and Liquid Droplet in Liquid Co-Flow.	MF-P26
27	Vivek Karma	An Experimental Study of Streaming Patterns Around an Acoustically Oscillating Single Air Bubble in Water	MF-P27
28	Arunachalam S	Drop breakage using inserts in two-phase systems	MF-P28
29	V.S. Anvesh Sangadi	Lightning Stokes Solver for wedge flows: application to moving contact lines	MF-P29
30	Arasakumaran K	Modelling the simultaneous entrainment of two liquids with slip	MF-P30
31	Ghanashyam K. C	Development of an electrohydrodynamic solver for polymer electrospinning and analytic modelling of an electrified jet subjected to insoluble surfactants.	MF-P31
32	Tejasvi Hegde, Rishabh Sharma	Experimental evidence of a slip near a moving contact line	MF-P32
33	Himanshu Mishra	Orientation dynamics of a settling spheroid in a simple shear flow	MF-P33

34	Namratha Kulkarni	Theoretical modelling of dark fringe formation during colorimetric detection of Pb using NaRh assay	MF-P34
35	Navin Kumar Chandra	Bag breakup of a polymeric droplet in a continuous flow air stream	MF-P35
36	Azim Memon	Simulation of Fluid-Particle suspension using the Immersed Boundary Method	MF-P37
37	Vaibhav Raj Singh Parmar	Stiffness-induced clustering of amphiphilic particles at air-water interface during drying	MF-P38
38	Kunal Kailash Sharma	Investigation of spin number and its influence on the cut-size in a spiral air jet mill geometry.	MF-P39
39	Ainkara Karthiga R	Effect of non-spherical drag on particle dynamics in fluidized bed - A CFD approach	MF-P40
40	Pallavi Katre	Ring formation in the Newtonian rod-climbing effect	MF-P41
41	Syed Shuja Hasan Zaidi	Surface-directed Spinodal Decomposition on chemically patterned substrate	MF-P42
42	Pramodt Srinivasula	Unexpected differences in the electrohydrodynamic oscillations of charged and polarized anchored water droplets	MF-P43
43	Shambhu Anil	Modelling dynamics of an Ultrasound Contrast Agent near a deformable wall using Kelvin Impulse	MF-P44
44	Malyadeep Bhattacharya	Improved surface tension force scheme for two-phase flow in diffuse interface framework	MF-P45
45	Swarnaditya Hazra	Entrapment of air-borne particles by pulmonary mucus films	MF-P46
46	Amitesh Kumar Chaudhary	Extensional rheology of polymer solutions for spray application	MF-P47

POLYMER AND HYDROGELS

ORAL PRESENTATION

POLYMERS AND HYDROGELS SESSION 1 - 18-12-2023

Time	Speaker	Title	Abstract ID
2:30 PM	Bhanu Nandan	Self-Assembly in Block Copolymer/Nanoparticle Mixtures	PH-O1
3:00 PM	Anindita Das	A Multifaceted Transesterification Route to Functional Polyesters	PH-O2
3:30 PM	Parbati Biswas	Intrinsic Viscosity and Rheology of Ring Polymers	PH-O3
4:30 PM	Swaminath Bharadwaj	Solvation Shell Thermodynamics of Extended Hydrophobic Solutes	PH-O4
5:00 PM	Ashok Kumar Dasmahapatra	Development of Conducting Polymer Nanocomposites for Energy Harvesting Applications	PH-O5
5:30 PM	Aritra Santra	Universality of dilute ring polymer solutions	PH-O6

POLYMERS AND HYDROGELS SESSION 2 - 19-12-2023

Time	Speaker	Title	Abstract ID
2:30 PM	Christopher Durning	Morphological Control During Polymer Crystallization	PH-O7
3:00 PM	Lenin S. Shagolsem	Collapse transition in a model heteropolymer: Effect of chain topology	PH-O8
3:30 PM	Shivalika Sharma	Low pH self-organisation of similarly charged Polyethylenimine chains into light-responsive microstructures.	PH-P33
3:45 PM	Ashima Choudhury	Pattern formation in electro-responsive polymer ionic liquid blends	PH-P21
5:30 PM	Rajdip Bandyopadhyaya	Local Drug Delivery to Pancreatic Tumor by Film and Gel-based Polymeric Implants	PH-O10

6:00 PM	Arindam Kundagram	Polymer complexation: Theory and application to the thermodynamics of complexation between highly charged disordered proteins	PH-O11
6:30 PM	Somesh Kurahatti	Simulation of Polyelectrolyte hydrogel Network with various charge densitities and network defects	PH-O12

POSTER PRESENTATION - 18-12-2023

Sl. No	Speaker	Title	Abstract ID
1	Banalata Kaibarta	Nanoclay based hierarchical mesoporous polyaniline/acetylene black nanocomposites for high energy density supercapacitors	PH-P1
2	Siddharth Saraswati	Structure-Property of Epoxy Blends in Electronic Packaging: Impact of Heating Rate	PH-P3
3	Prabeen Kumar Pattnayak	Diffusion of star polymers in dilute solutions: role of shape anisotropy	PH-P4
4	Devendra Kumar Verma	Phase separation kinetics of miktoarm star polymer in solvent: A DPD simulation study	PH-P5
5	Mounika Gosika	On the structure-viscoelasticity relationship of reversible polymer networks	PH-P8
6	Imran Hussain	Benzene tetracarboxylic acid doped polyaniline functionalized with graphene oxide: morphological and electrochemical characterization	PH-P9
7	Jagat Singh	Self-assembly of A2B Miktoarm Star Block Copolymer under Cylindrical and Spherical Confinements	PH-P12
8	Somtirtha Santra	Role of sequence on the phase behavior of thermoresponsive copolymers	PH-P13
9	Aathira Murali	Interaction of chitosan with water vapor: An experimental & simulation study.	PH-P14

10	Manish Dwivedi	Polymer translocation : Effects of confinement	PH-P15
11	Vishal Kumar	Combined Electromechanically Driven Pulsating Flow of Non-Linear Viscoelastic Fluids In Narrow Confinements	PH-P16
12	Viney Ghai	Role of Rheology on the Magnetic Field Orientation of Graphene Nanosheets in Polymers	PH-P17
13	Tushar Mahendrakar	Comparisons between Free Monomer Clusters and Polymer Globules by using Molecular Simulations	PH-P18
14	Sateesh Kumar Gupta	Influence of Ca2+ Ions on Rheological and Dielectric Behavior of Sodium Carboxymethyl Cellulose (NaCMC) and Esterified Hydrogels	PH-P19
15	Shinjini Das	Salt-dependent swelling kinetics of polyelectrolyte gels	PH-P20
16	Ashima Choudhury	Pattern formation in electro-responsive polymer ionic liquid blends	PH-P21
17	Vrinda Garg	Dynamics of interior loop formation in polymer chains: effect of tail length and confinement	PH-P22
18	Sumitra Rudra	Thermal melting and force induced unzipping of DNA hairpin: Unfolding pathways and phase diagrams	PH-P23
19	Sayani Karmakar	Predicting Phase Behavior of Polymer-Nanorod Composites Via Coarse-Grained Molecular Dynamics Simulations	PH-P24
20	Swasthika Arunachalam	Investigation of cone shape parameters in polymer electrospinning via in situ visualization: towards precise control over fiber diameter	PH-P26
21	Anagha C R	Improving functional Properties of PNIPAM hydrogel using extracted seed mucilage of Salvia Hispanica	PH-P27

22	Shakshi Gupta	Novel Evaporation Kinetics of a Droplet Containing Polymer	PH-P28
23	Manoj Kumar Maurya	Tuning Thermal conductivity in bottlebrushes: A molecular dynamics simulation approach	PH-P29
24	Vivek Sharma	Polyethylene grafted sheet-like silsesquioxane nanocomposites with unprecedented adhesion to polar substrates	PH-P30
25	Krithika Bhaskaran	Rheological studies on seed mucilage layers	PH-P31
26	Projesh Kumar Roy	Soft and adhesive alginate hydrogel: Microstructure from MD simulations	PH-P32
27	Shivalika Sharma	Low pH self-organisation of similarly charged Polyethylenimine chains into light-responsive microstructures.	PH-P33
28	Amit Yadav	Spreading and Evaporation of a Polymeric Droplet Impacting on Nonporous Substrate	PH-P34
29	BALAAJI M	Particle image velocimetry as a tool to investigate lubricating effect of root mucilage	PH-P35
30	Sharanya Alluri	Predicting Mechanical Properties of Biodegradable Copolymers using Molecular Dynamics Simulations	PH-P36
31	Ravi Kumar Pujala	Novel composite hydrogels with enhanced thermal stability and injectability	PH-P37
32	Keerthi Radhakrishnan	Adsorption of pH responsive ampholytic ions into a weak PE brush: A simulation study	PH-P39
33	Vijith S	Effect of Degree of Confinement on Mechanical Properties of Polymers Through Free Volume.	PH-P40
34	Smruti Parimita	Solvent-assisted ink-based 3D printing of free-form structures via phase separation	PH-P41

RESPONSIVE SOFT MATTER

ORAL PRESENTATION

RESPONSIVE SOFT MATTER - 18-12-2023

Time	Speaker	Title	Abstract ID
9:00 AM	Pijush Ghosh	pH Responsive Actuators: Controlling Actuation Direction & Printing	RS-O4
9:30 AM	Umadevi	Liquid crystal elastomer-based soft actuators	RS-O1
10:00 AM	Himangsu Bhaumik	Material Training through Mechanical Regularization	RS-O3
11:00 AM	Apala Majumdar	Tunable Textures in Cholesteric Liquid Crystal Shells for Sensing and Other Applications	RS-O5
11:30 AM	Raj Kumar Roy	Understanding the role of polyproline's secondary structures in thermal phase transitions and bulk phase separations	RS-O6
12:00 PM	Subrata Chattopadhyay	Reactive stimuli-responsive poly(aminoamide) microgels as a platform for diverse sensing applications	RS-O2

POSTER PRESENTATION - 18-12-2023

Sl. No	Speaker	Title	Abstract ID
1	Ashish Kumar Singh	A DPD study on the impact of external shear due to moving rigid walls, on the phase separation dynamics of polymer fluids	RS-P1
2	Kushal Bagchi	Preparing functional soft materials through the directed self-assembly of complex liquid crystals	RS-P2
3	Saikat Das	Topological defects and electrokinetics of emulsion droplets in nematic liquid crystals	RS-P3

4	Rahul Karmakar	Hot crystals of thermo-responsive particles with temperature dependent diameter in the presence of a temperature gradient	RS-P4
5	Kalyani Agarwal	Nucleation of Bulk Nanobubbles During Oscillating Pressure Field	RS-P5
6	Archana S	Transport of magnetodielectric particle in a nematic liquid crystal under transverse electromagnetic fields	RS-P6
7	Satyendra Rajput	Ethylene glycol energetically destabilizes aggregates of pseudoisocyanine dyestuffs at crowded concentrations	RS-P7
8	Vipin Kumar	Controlled actuation of gelatin based soft actuators in response to multiple vapor	RS-P10
9	Sarah Ahmad Siraj	Vapor-responsive tunable actuation of silk films: Effect of secondary structures	RS-P11
10	Abinash Barthakur		RS-P12
11	Rajesh Pavan Pothukuchi	Understanding The Role Of Shape-Dependent Anisotropy Of Electrostatically Driven Nanoparticle Self-Assembly	RS-P13
12	Akash Patil	Coupled Photo-Mechanics of Nematic Liquid Crystal Elastomers - An ABAQUS UEL Implementation	RS-P14
13	Prasoona Rani	Effect of Counterions on Polyelectrolytes: A Molecular Dynamics Simulation Study	RS-P15
14	Surbhi Khewle	Role of interfacial properties on the mechanical deformation in light-activated polymer blends	RS-P16
15	Neeraj C. S.	Multi-dye-based light/thermal responsive liquid crystal polymer films	RS-P17
16	Sanghamitra Debta	Numerical Investigation of Coupled Swelling-Deformation Behavior of Functionally Graded Hydrogel Thin Films	RS-P18

17	Sachin Singh Rajput	Computational validation of stimulus-responsive anisotropic PVDF film	RS-P19
18	P.S. Patwal	Buoyancy-driven microgel oscillator: Beating and Bouncing dynamics	RS-P20
19	Sayantan Chanda	Studying the effect on yielding behaviour of dense suspensions of thermo-responsive PNIPAM particles by tuning inter-particle interactions	RS-P21

RHEOLOGY AND CONSTITUTIVE MODELLING

ORAL PRESENTATION

RHEOLOGY AND CONSTITUTIVE MODELLING -20-12-2023

Time	Speaker	Title	Abstract ID
2:00 PM	Ravi Kumar Pujala	Novel composite hydrogels with enhanced thermal stability and injectibility	RC-O1
2:30 PM	V. Shanker	Role of finite extensibility on the center-mode instability in viscoelastic channel flow	RC-O2
3:00 PM	Naveena C S	The linear and nonlinear rheological characteristics of the biofilm formed by Mycobacterium Smegmatis	RC-O3
3:15 PM	Puchalapalli Saveri	Tuning the non-linear rheological response of low molecular weight supramolecular gels	RC-O4
4:00 PM	Luca Cipelleti	A unified state diagram for the yielding transition of soft colloids	RC-O5
4:30 PM	Mahesh Ganesan	Fractional calculus derived empirical predictive relations for the linear viscoelasticity of semi-dilute polymer solutions	RC-O6
5:00 PM	Balaji Iyer	Modeling Local and Collective Dynamics in Polymer Grafted Nanoparticle Systems	RC-O7

POSTER PRESENTATION - 19-12-2023

Sl. No	Speaker	Title	Abstract ID
1	Shivi Garg	Single contaminated droplet microextraction in a yield-stress fluid	RC - P1
2	Anaswara Das K	Non-equilibrium dielectric relaxation of a nematic liquid crystal	RC - P2
3	Sachin M B Gautham	Non-Linear Rheology of Polymer Grafted Nanoparticle Solutions	RC - P3
4	Anant Chauhan	Effect of geometric disorder on chaotic viscoelastic porous media flows	RC - P4
5	Surya Phani Tej Pulakhandam	Purely Elastic Center mode Instability in Dean Flow	RC - P5
6	Shailendra Kumar Yadav	Elastic center-mode instability in viscoelastic plane Couette-Poiseuille flow	RC - P9
7	Vivek Kumar	Rheological Behavior of Colloidal Silica Gel	RC - P14
8	Naved Khan	Fractional calculus derived empirical predictive relations for the linear viscoelasticity of semi-dilute polymer solutions	RC - P15
9	Naveen Kumar Agrawal	Novel Periodic Shear Protocols: Understanding Rheology and RIT	RC - P16
10	Abhishek Ghadai	Flow around a local probe driven in wormlike micelles: origin of flow instabilities	RC - P17
11	Gunjan Sharma	Unveiling the enhanced magnetorheo-transport dynamics in magnetic ionic liquid	RC - P18

12	Raviteja Miriyala	First normal stress differences in TEVP fluids	RC - P19
13	Faraz A. Burni	An organogel programmed to spontaneously degrade: How a breakthrough in rheology can enhance oil production	RC - P20
14	Ishu Chaudhary	Insights on Slip-layer Dynamics Using Electrorheology	RC - P21
15	Saurabh Maurya	Numerical simulations for electro-osmotic flow of PTT fluids in diverging microchannel	RC - P22
16	Sankata Tiwari	Rheological behaviour of Aqueous alumina suspension for Direct Ink writing process	RC - P23
17	Isha Misra	Dynamics of spherical particles in the presence of shear and oscillating magnetic field	RC - P24
18	Anupama Gannavarapu	Effects of local incompressibility on the rheology of composite biopolymer networks	RC - P26
19	Shrajesh Patel	Physical Aging Behavior of Aqueous Solution of Pluronic F127	RC-P27
20	Catherine Sanchana	Use of multi-wave rheological technique to characterise bitumen at low	RC-P28
21	Greena Maria Sunny	Influence of Frequency and Temperature on Warping Stress in Bituminous Mixture	RC-P29
22	Thirumalavenkatesh Medem	Apparent viscosity and shear rate dependency characterization of reclaimed asphalt pavement (RAP) binders	RC-P30
23	Atanu Behera	Investigation of the Various Relaxation Modes for a Class of Bituminous Mixtures	RC-31

24	L. Abinaya	On the Arrhenius response of aged bituminous binders	RC-32

SURFACTANTS AND MEMBRANES

ORAL PRESENTATION

SURFACTANT AND MEMBRANES - 20-12-2023

Time	Speaker	Title	Abstract ID
2:00 PM	Srinivasa Raghavan	Extending self-assembly beyond water: Wormlike micelles and vesicles in polar solvents at sub-zero temperatures	SM- O6
2:30 PM	Samapika Sahu	Unveiling Guest Molecule induced Alterations in model membranes	SM - O1
3:00 PM	Hirak Chakraborty	Protein machines and lipid assemblies: interdependence in membrane fusion	SM - O4
4:00 PM	Sajal Kumar Ghosh	Assembling of DNA macromolecules at air-water interface	SM -O2
4:30 PM	Durba Sengupta	Interactions of cellular metabolites with membranes	SM-O5
5:00 PM	Jyoti Gupta	Unraveling Interactions between Ionic Liquid and DPPC Membrane	SM-P16

POSTER PRESENTATION - 19-12-2023

Sl. No	Speaker	Title	Abstract ID
1	Ajit Seth	Self-assembly of graphene-based nano-materials in and around a lipid film	SM-P1
2	Devansh Kaushik	Modified structure and physical properties of a model lipid membrane caused by an Antidepressant Drug	SM-P3
3	Prashanta Swain	Computational Microscopy of Cyclodextrins - Membrane Interactions	SM-P4
4	Prateek Chowdhury	Influence of SAM Growth on Wetting: Insights from Mass-Transfer Models	SM-P5
5	Renu Saini	Aggregation of chlorophylls on plant thylakoid membranes using coarse-grained simulations	SM-P6

6	Nalinikanta Behera	Electroporated-deformation of vesicles under ms-pulsed electric field	SM-P7
7	Sivadas P	Probing mechanism of membrane activity for small molecule based sequence defined oligomers	SM-P8
8	Vidhya Vijayakumar	Techniques for Low temperature Demulsification of Pickering Emulsion	SM-P9
9	Nithya M	Nisin-lipid bilayer interactions: A study on the kinetics of pore formation in vesicle membrane	SM-P10
10	Kailash Veerappan Uma Kumar	Spreading and Imbibition of Structured fluids on Porous Substrates	SM-P11
11	Rupesh Kumar1	Electrodeformation and dye leakage study of Giant Unilamellar vesicles (GUVs) under DC and AC electric field Pulses	SM-P14
12	D.Mahesh	Structure and Dynamics of Polymer Tethered Nanocomposites in Bulk and Interfaces	SM-P15
13	Md Rashid Ali Faridi1	Understanding electrostimulation of neurons without electroporation	SM-P17
14	Manaswini Gowtham V	Interactions between similarly charged surfactants & nanoparticles – effect of size and geometry	SM-P18
15	Chetan TBV	Effect of Dissolved Polymer and Surfactant on the Evaporation of a Liquid Bridge	SM-P19

SUSTAINABILITY

ORAL PRESENTATION

Sustainability - 20-12-2023

Time	Speaker	Title	Abstract ID
2:00 PM	Janani Sampath	Gas transport through amorphous polymer membranes from all-atom molecular dynamics simulations	SU-O1
2:30 PM	Thi Vo	Leveraging Stimuli-Responsive and Reconfigurable Block Polymers for Sustainable Materials Design	SU-O2
3:00 PM	Santosh Kumar	Flexible Thermoelectric Films Produced via Printing for Energy Harvesting Applications	SU-O3
3:15 PM	Sreejith Chakrapani	Production Of Polystyrene Microparticles Using Glass Modular Microfluidic Device (MMFD)	SU-O4
4:00 PM	Sanat Kumar	Nanoplastic Formation Mechanisms	SU-O5
4:30 PM	Tarak Patra	Modeling Compatibilization of Mixed Plastic Wastes	SU-O6
5:00 PM	Guruswamy Kumaraswamy	Unprecedented adhesion of polyethylene-grafted sheetlike silsesquioxanes	SU-O7

POSTER PRESENTATION - 18-12-2023

Sl. No	Speaker	Title	Abstract ID
1	Javed Akhtar	Modeling Catalytic Degradation Mechanism of Polymers Using Density Functional Theory	SU-P1
2	Ganesh Kumar Rajahmundry	Predicting Percolation Phase Behaviour of Polymer Electrolytes using Coarse-Grained Molecular Simulation	SU-P3
3	Somas Singh Urikhinbam	Conductivity of a Size Polydispersed Ionic Liquid: A Molecular Dynamics Simulation Study	SU - P4
4	Mantosh Kumar Yadav	Development of Polymer/Composite based Growing Chamber with Controlled Temperature for Soil-less Agritech	SU-P5

TABLE TALKS

TABLE TALK SESSION 1 (19-12-2023)

Time	Speaker	Title	Abstract ID
2.30 PM - 3.30 PM	Mithun Radhakrishna	Investigating the Chaperone Mechanism of α-Crystallin in Preventing γDCrystallin Aggregation in Cataract Formation	T1-01
	Satyavrata Samavedi	Designing functional electrospun matrices: from polymer physics to biomedical applications	T1-02
	Athi Naganathan	Proteins, Strings, and Mechanisms	T1-03
	Hamsa Priya	Tracing Solvent Hydrogen Bond Network Reveals Surprising Facts	T1 -04
	Sharad Gupta	Homocitrulline-containing peptide amphiphiles: Amyloids or Coacervates?	T1-05

TABLE TALK SESSION 2 (19-12-2023)

Time	Speaker	Title	Abstract ID
2.30 PM - 3.30 PM	Ronald Benjamin	Efficiency of an Active Brownian particle in a ratchet potential	T2-01
	Alan R Jacob	Towards developing sustainable fat substitutes	T2-02
	Parag Ravindran	A discussion on a few models for Thixotropic fluids	T2-03
	Bidisha Sinha	Regulation and role of plasma membrane mechanics in adherent cells	T2-04

	Indranil Saha	The FENE-mode model to accurately predict temporal variations of configuration and stress of polymer chains in solutions	T2-05

TABLE TALK SESSION 3 (19-12-2023)

Time	**Speaker**	**Title**	**Abstract ID**
5.30 PM - 7.00 PM	Swapna Singha Rabha	Multiphase Flow and Flow in Porous Media for Energy Applications	T3-01
	Harish Dixit	Moving Contact Lines: singularity, flow fields, and new insights from experiments	T3-02
	Anki Reddy Katha	Insights into water-salt dynamics in polyamide and graphene oxide-based membranes and protein-surface interactions via computational approaches	T3-03
	Kiran Raj	Soft matter biomicrofluidics – from mimicking blood flows to cancer drug screening	T3-04
	Gaurav Tomar	Numerical Modeling of Capsules in Microchannel Flows	T3-05
	Himanshu Goyal	Modeling multiphase reactors for clean energy	T3-06

TABLE TALK SESSION 4 (19-12-2023)

Time	**Speaker**	**Title**	**Abstract ID**
	Nirmalya Bachhar	Understanding the effect of Methyl group of molecules in polymer solutions	T4-01

5.30 PM - 7.00 PM	Sivasurender Chandran	Pattern Formation in thin films of evaporating polymeric solutions – an interplay between evaporation and spreading rate	T4-02
	Susy Varughese	-	-
	Deepak Arora	Polymers for Advanced and Sustainable Manufacturing	T3-04
	Omkar Deshmukh	Understanding Mucin-Albumin assembly using microrheology	T3-05
	Kamendra Sharma	Ultra-sensitive protein detection at the aqueous-liquid droplet interface using microfluidic engineering and accoustic patterning	T3-06

THIN FILMS & POLYMER MEMBRANES

ORAL PRESENTATION

THIN FILMS AND POLYMER MEMBRANES - 19-12-2023

Time	Speaker	Title	Abstract ID
9:00 AM	Jaydeep Basu	Enhanced efficiency of water desalination in nanostructured thin-film membranes with polymer grafted nanoparticles	TP-O4
9:30 AM	Deepak Kumar	Peeling a thin sheet from a liquid surface	TP - O6
10:00 AM	Simone Napolitano	Equilibration pathways beyond density fluctuations: the Slow Arrhenius Process	TP - O5
11:00 AM	Marcus Mueller	Fabrication of block co-polymer membranes:what can be learned from the coarse grain models?	TP - O1
11:30 AM	Ateeque Malani	Structure of adsobed water present on thin film mica membranes: effect of exposed ions	TP - P18
12:00 PM	Satish Sukumaran	Using swelling of polymer thin films to investigate the tightly bound layer at a polymer/substrate interface	TP - O3

POSTER PRESENTATION - 19-12-2023

Sl. No	Speaker	Title	Abstract ID
1	Jyothi Priya Sarkar	Role of nanoparticle architecture and polymer-nanoparticle interface in unconventional flow of polystyrene thin films	TP - P1
2	Bharti	Rayleigh-Plateau Instability of a Viscoelastic Layer Coated on a Rigid Cylindrical Fiber	TP - P2
3	Patel YogeshKumar DalpatBhai	Effects of monomer sequence on the gas sorption and diffusion in a copolymer membrane	TP - P3

4	Yogitha Maithani	LIG coated Flexible and Reusable Textile based Dry Electrodes for Biopotential Sensing	TP - P4
5	Mahrukh Arif Mir	Smearing Technique For Liquid Viscosity Measurement	TP - P5
6	Pankaj Mahawar	Viscoelastic Bursting of Spin Coated Polymer Surfaces	TP - P6
7	Moirangthem Prem Meitei	Charged diblock copolymer melts under shear: A molecular dynamics simulation study	TP - P7
8	Shreyanil Bhuyan	Linear stability analysis of a thin film of polar polymer solutions	TP - P8
9	Ashish Biswas	Entropic and Enthalpic effect on interfacial jamming in polymer blend nanocomposite BIJELS	TP - P9
10	Ramya Durga Manga	Numerical study of instability ferrofluid thin film using hybrid lattice Boltzmann method	TP - P10
11	Sonam Zangpho Bhutia	Investigation of Bound Layers in Thin Films of Hydrophilic Polymers and Their Nanocomposites	TP - P11
12	Ratnadeep Samanta	Banana leaf inspired anisotropic slippery surfaces	TP - P12
13	Sudeshna Dhar	Effect of Plasticizer on Dewetting and Crazing Dynamics of Poly(p-tertbutylstyrene) Thin Films	TP - P13
14	Harshit Yadav	Structure and water transport through block copolymers with a sulfonated hydrophilic block	TP - P14
15	Igin Benny Ignatius	The effect of parametric forcing on the supercritical Marangoni instability	TP - P16
16	Chiranjith Majhi	Effects of externally deposited nanoscale heterogeneities in thin polymer films on their interfacial behaviors	TP - P17
17	Shreyank Goel	A reduced-order model for surfactant-laden electrified sessile droplets	

AM - O10

Collapse Dynamics of Flexible Active Polymer

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The active matter systems feature the perpetual conversion of chemical energy or other forms of energy into mechanical motion that drives the system out-of-equilibrium. In this work, we are interested in studying one particular branch of such active systems, that is the active polymer which exhibits various interesting dynamics like self-propulsion, swelling, shrinkage, loop formation, spontaneous oscillation, spiral formations, enhanced diffusion etc. The linear and circular structures in many synthetic or natural systems simultaneously experience local and long-range forces. In this work, we use numerical simulations to investigate the concurrent effect of a local polar and attractive long-range activity on the active polymer. The source of activity on the polymer is the self-generating, nonequilibrium solvent gradient caused by the chemical reaction at different sites on the polymer. The chemical gradient then leads to the generation of both local and long-range force along the filament. Here we present the effect of activity on the configurational dynamics of a flexible chain emphasizing globulelike transformation for linear topology. However for rings, while the long-range attraction leads to a systematic collapse, the polar activity tends to swell the shorter rings and crumple the larger ones. We show that the steady-state conformation of such an active ring strongly depends on the kind of activity. The dominance of local tangential activity for very short rings, while the long-range activity at intermediate length scales is observed. However, in contrast to our intuition, we observe the dominance of local polar activity again for very large rings. We quantify these observations by comparing the scaling laws and local structures with the passive polymers. Further, the relaxation dynamics of the polymer were characterized by the Rg, and a nonmonotonic behavior was observed for polar activity for rings.

Indian Society of Rheology

Active Matter with Robots

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In this talk, I will present a novel robotic active matter system developed in our lab. It consists of macroscopic programmable self-propelled differential-drive robots equipped with hardware components like IR and light intensity sensors (see Fig. 1) that enable them to detect obstacles and react to external optical signals. I will present simple protocols to program the robot to exhibit various scalar active particle models with excellent agreement with theoretical predictions [1]. Later, I will show some ongoing experimental findings related to the collective behavior of these robots coupled to each other through rigid rods. Finally, I will show how this robotic system can be adapted to mimic the fascinating features of complex living systems, which may help us better understand these systems physically.

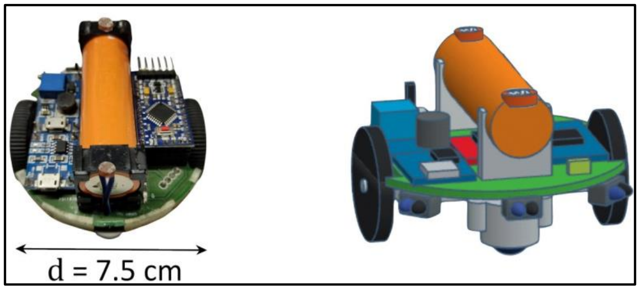

Figure 1: Arduino-based programmable robots. They use the differential drive mechanism such that each wheel moves independently, providing high maneuverability.

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AM - O7

Indian Society of Rheology

An active particle at a soft interface

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The motion of a passive Brownian particle is a manifestation of equilibrium thermal fluctuations. On the other hand, active particles which are self-propelled are capable of taking energy from the environment and converting it into directed motion. The active particles moving in a homogeneous environment without physical confinements have been investigated both theoretically and experimentally. However, the effect of confinement on active particle dynamics is an emerging area of research due to its relevance to biological systems. We have investigated the effect of soft boundaries on the Brownian dynamics of active particles. In this talk we will discuss some of our recent results obtained from confined natural active particles

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AM - O3

Bioinspired Soft Matter Using Solitons in Liquid Crystals

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Non-equilibrium states of soft matter that form via the dissipation of energy form the basis of many biological processes central to life (e.g., cell division). Such states of matter often arise from highly non-linear phenomena that generate a strongly localized response to a delocalized stimulus. Solitons in liquid crystals (LCs) represent one such class of non-linear phenomena with the potential to provide fundamental insight into the transfer of energy, chemical species and information that has been observed to accompany solitons in biological and synthetic soft matter. Solitons are highly confined, propagating waves that arise from non-linear feedback in natural (e.g., shallow and confined waters) and engineered systems (e.g., optical wave propagation in fibers). In the context of LC films, dissipative solitons are observed as highly localized and rapidly propagating LC director orientational responses that are triggered by external fields. In this talk, we will first discuss the recent advances which have unmasked the central role of surface chemistry in programming the formation and propagation of these structures. We will also demonstrate how patterned anchoring of LCs permits control over soliton formation and trajectories via the complex behaviors of solitons at discontinuous LC domain boundaries. Finally, aided by recent computational studies, which have deconstructed the associated energetics, we will show how solitons in LCs can be used to focus the energy of non-localized electric fields to generate a new class of non-linear electrohydrodynamic effects at fluid interfaces, including jetting and emulsification. Overall, these works suggest that solitons in LCs offer exciting opportunities to achieve new forms of active matter enabling energy transduction and accelerated transport processes.

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AM - O5

Microscopic Gyration With Dissipative Coupling

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Microscopic gyrator including Brownian gyrators (BGs), require anisotropic fluctuations to perform gyration. It produces a finite current, driving the system out of equilibrium. In a typical BG set-up with an isotropic colloidal particle, the anisotropy sets in by the coupling among space dimensions via an externally applied anisotropic potential confining the particle and the difference between the temperatures along the space dimensions. The coupling is conservative. Here, contrary to a typical BG, first we consider an over-damped, anisotropic colloidal particle (a Brownian ellipsoid), trapped in an isotropic harmonic potential in two dimensions (2D). The trapping potential being isotropic, cannot couple the space dimensions. Instead, they are coupled by the difference between the longitudinal and transverse frictional drags experienced by the ellipsoid, together with a finite tilt in its orientation due to the chirality of the particle. The coupling can not be derived from a potential. It is dissipative. It is associated with the intrinsic properties of the particle. We have shown that the dissipative coupling can generate enough anisotropic fluctuation to perform a steady-state gyration in the Brownian scale. Next, going beyond BG, we have considered an inertial, granular, chiral ellipsoid in 2D, subjected to athermal, anisotropic fluctuation. Unlike BG, there is no trapping force confining the granular ellipsoid. However, the coupling between the velocity components of the granular ellipsoid is still dissipative. We have shown that being assisted by the dissipative coupling and the anisotropic fluctuations, the inertial, granular ellipsoid can also perform gyration in 2D. Furthermore, we have shown that the dominant contribution towards the gyration is attributed to the Coriolis force acting on the granular ellipsoid. Hence, similar to the Brownian scale, the gyrator in the granular scale is also a tiny autonomous machine that generates a directed motion (gyration) from fluctuations.

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AM - O6

Phase separation of passive particles in active liquids

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The transport properties of colloidal particles in active liquids have been studied extensively. It has led to a deeper understanding of the interactions between passive and active particles. However, the phase behavior of colloidal particles in active media has received little attention. We have studied passive colloids dispersed in suspensions of active particles in experiments and simulations. Our study reveals dynamic clustering of colloids in active media due to an interplay of active noise and an attractive effective potential between the colloids. The size-ratio of colloidal particles to the bacteria sets the strength of the interaction. As the relative size of the colloids increases, the effective potential becomes stronger and the average size of the clusters grows. The simulations reveal a macroscopic phase separation of passive colloids at sufficiently large size-ratios. We will present the role of density fluctuations in the emergence of effective interactions.

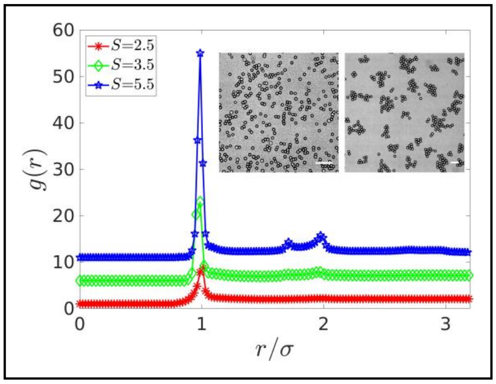

Figure 1: Clustering of passive colloids in active liquids. The size of the clusters increases with increasing size ratio (S) of the colloids and bacterium.

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AM - P18

Indian Society of Rheology

How viscoelasticity influences the orbital dynamics, microstructure and rheology of dilute active suspensions

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The localized energy-work conversion of active microswimmers has been known to impart anomalous macroscale properties in stark contrast to passive suspensions. Recent experiments have measured viscosity reduction to a near-zero limit in the steady-shear flow of Newtonian fluids. Motivated by the ubiquitous microbial systems in biological fluids, we theoretically analyse the departure from Newtonian assumptions: how weak viscoelasticity can alter the rheological response of active spheroidal suspensions. At the individual level, orientations of the elongated swimmers follow the well-known Jeffery orbits in Newtonian shear flows, identical to the passive particles. We find that activity makes a difference when fluid is viscoelastic: passive particles are long-known to exhibit log-rolling orbits, which are altered when particles shed active disturbances (Fig. 1). To analyze its impact on the bulk rheological response, we study a dilute ensemble of microswimmers in the presence of stochastic noise from tumbling and rotary diffusion. Compared to Newtonian media, activity in polymeric media further amplifies the swimmer-induced viscosity modifications in a manner that scales quadratic to swimmer's persistence length.

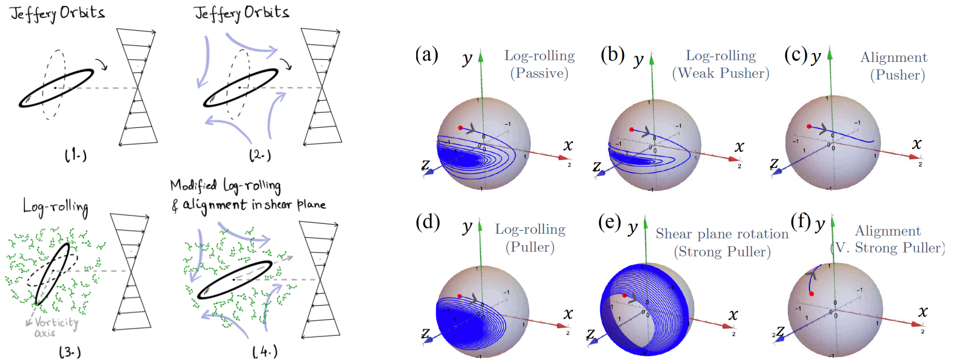

Figure 1: [Left] Schematic illustrating the effect of activity in Newtonian and viscoelastic shear. [Right] Results on orientational dynamics: In viscoelastic fluids, passive particles exhibit a slow drift to a log-rolling state. E. coli type swimmers (pushers) are found to affect this log-rolling opposite to that by C. reinhardtii (pullers), where the former can even achieve alignment at low to moderate activity.

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AM - O4

Swimming Efficiently by Wrapping

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Single flagellated bacteria are ubiquitous in nature. They exhibit various swimming modes using their flagella to explore complex surroundings such as soil and porous polymer networks. Some single-flagellated bacteria swim with two distinct modes, one with its flagellum extended away from its body and another with its flagellum wrapped around it. The wrapped mode has been observed when the bacteria swim under tight confinements or in highly viscous polymeric melts. In this study we investigate the hydrodynamics of these two modes inside a circular pipe. We find that the wrap mode is slower than the extended mode in bulk but more efficient under strong confinement due to a hydrodynamic increase of its flagellum translation-rotation coupling.

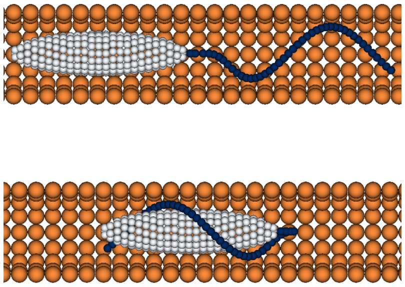

Figure 1: Bacteria inside a pipe with its flagellum in the extended and wrapped modes

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Indian Society of Rheology

Characteristic features of self-avoiding active polymers under shear flow

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In this talk we are going to present Brownian dynamics simulation results of a self-avoiding flexible polymer chain under linear shear flow in the presence of active noise. The active noise strongly affects the polymer conformational and dynamical properties under shear flow, such as the stretching in flow direction and compression in the gradient direction, shear-induced-alignment, and shear viscosity, and in the asymptotic limit of large activities and shear rates, their power-law scaling exponents differ significantly from that of passive chains. The compression of the active chain in the gradient direction follows the relation $\sim Wi_{Pe}^{-2/3}$ as a function of the activity-dependent Weissenberg number Wi_{Pe}, which differs from the scaling observed in passive systems $\sim Wi_{Pe}^{-1/2}$.[2] The flow-induced alignment at large shear rates $Pe >> 1$, where Pe is the P'eclet number, and large $Wi_{Pe} << 1$, displays the scaling behavior $Wi_{Pe}^{-1/3}$, with an exponent differing from the passive value $1/2$. Furthermore, the polymer's zero-shear viscosity displays a non-monotonic behavior, decreasing in an intermediate activity regime and increasing again for large Pe induced by excluded-volume interactions. The shear viscosity is found to decrease with the Weissenberg number following the power-law relation $Wi_{Pe}^{-\beta}$, where $\beta = 1/2$[3,4] and $\beta = 2/3$ for passive and active polymers, respectively. In addition, our simulation results are compared with the results of an analytical $model$[1,5], which predicts quantitively similar behaviors for the various aforementioned physical quantities. Additionally, we show the results of the active polymer when the chain is driven by a tangentially active force whose direction is along the bonds of the chain. In such a scenario, the various scaling exponents differ dramatically. In both cases the structural dynamics is will be very different from its passive counterpart.

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Indian Society of Rheology

Sculpting vesicles with active particles: Less is more

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Biological systems are fascinating examples of soft matter, capable of processing both chemical and mechanical information while actively responding to internal and external cues [1]. One of the paramount challenges in modern science is understanding cellular self-organization and function, and subsequently reconstituting the basic principles of life. In this pursuit, engineering simple cell-mimicking systems provides an opportunity not only to gain insights into their more complex natural counterparts but also to derive design principles for soft functional micro-robots capable of performing cell-like and beyond-nature tasks.

In this presentation, I will introduce a simplified biomimetic system designed to investigate how the cell membrane responds to highly localized forces, such as those originating from the cytoskeleton or intercellular bacteria like listeria. In our system, the cell membrane is mimicked by giant unilamellar vesicles of lipid bilayers and the local internal forces are generated by enclosing self-propelled particles [2]. I will demonstrate that propulsion forces as small as ~0.1 pN are sufficient to significantly distort the shape of these vesicles, leading to active membrane fluctuations. Our research provides a foundation for understanding the relationship between localized active forces and dynamic changes in vesicle shape [3].

Additionally, I will discuss how control over endocytosis pathways can be achieved by carefully manipulating curvature, shape, and the adhesive force between particles and the lipid membrane [4]. These findings advance our understanding of cellular shape dynamics and have practical applications, not only in the design of artificial systems like soft micro-robots and synthetic cells but also in the development of targeted drug delivery methods.

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AM - P46

How do activity and inertia control non-equilibrium features of active Brownian particles?

Manish Patel[1], Shubendu Khali[1], Fernando Peruani[2], Debasish Chaudhuri[*,1],
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We will consider inertial active particles acted on simultaneously by Brownian and active noise. We present a direct method to derive exact expressions for all moments of dynamical variables in arbitrary dimensions. The analytic results are verified against numerical simulations and used to analyze interesting dynamic crossovers. Using illustrative examples, we will show how an interplay of activity, stiffness of external trapping potential, and inertia leads to dynamic crossovers between equilibrium-like and purely non-equilibrium distributions [1]. In the presence of excluded volume interactions, remarkable new features arise — the steady-state diffusivity and mobility of a tagged particle decrease with mass [2]. These many-body results are rationalized using kinetic theory arguments.

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How turnover triggers nonlinear waves in the active actomyosin cortex

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Below the plasma membrane of every eukaryotic cell resides a thin layer of active gel called the actomyosin cortex. This meshwork of actin filaments and myosin molecular motors is the site of fascinating self-organized patterns of forces and flows that control cell division and polarity, as well as morphogenetic processes at the tissue scale [1]. The fundamental mechanochemical feedback---*active* myosin motors generate contractile forces within the cortex which drive flows that in turn redistribute the myosin---may be described by a simple one dimensional model consisting of an advection-diffusion equation for the concentration of an active stress regulator (myosin) and the Stokes flow equation [2]. While this model gives rise to stationary patterned states via a linear instability, it has hitherto been thought that it is insufficient to explain the wave-like patterns observed in experiments [1,3], and that one must introduce additional complexity, such as a second biochemical species or cortical elasticity [3]. In this work, we show and explain how the inclusion of a simple linear reaction, which models turnover of material in the cortex, can surprisingly trigger the onset of waves. While such single-active-species waves have been observed previously [4], we here carryout extensive simulations (Fig. 1) and thereby (i) show that these waves arise via a secondary bifurcation but only when the turnover rate (R) is non-zero, and (ii) reveal how the critical value of the active stress strength (Pe) depends on the turnover and cortical viscosity. We also explain the key role played by turnover in triggering these waves, by drawing insights from a reduced-order Galerkin-truncated ODE model. The waves are found to be a robust feature of the dynamics, arising in both one and two dimensional domains, with either periodic or no-flux boundaries.

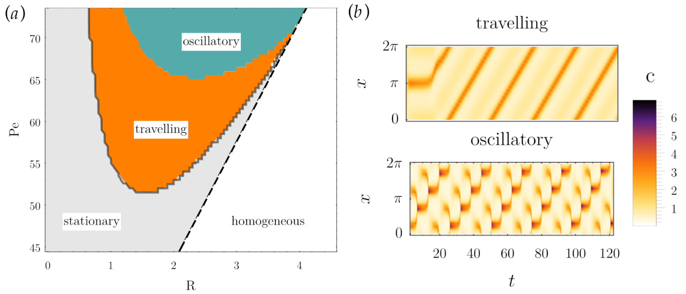

Figure 1: Regime map showing the emergence of travelling and oscillatory waves in the Pe - R parameter plane. (b) Space-time plots of the travelling waves (top panel) and modulated or oscillatory travelling waves (bottom panel).

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AM - P38

Controlled dynamics of microbes in confinements: how to exploit shape and flexibility

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Understanding the dynamics of microbes in confined flow channels is sought after for several medical and biotechnological applications. I will present our recent theoretical work predicting how we can exploit the shape and flexibility of the microswimmers and control their dynamics under confinements using the imposed conditions. We study a flagellated microswimmer with flexible tails and develop the complex hydrodynamics coupling the self-propulsion and active flows. Our results show remarkable consequences of shape and flexibility resulting in a rich non-linear dynamic. I will present our analysis examining the key factors governing the observed behaviors of the microswimmers under confinements.

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AM - P6

Emergent rigidity in chemically self-interacting active polymers

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We model the ith active droplet as a colloid particle centered at $\boldsymbol{R}_i$, confined to move in two-dimensions, which self-propels with a speed v_s, along the directions $\boldsymbol{e}_i = (\cos\theta_i, \sin\theta_i)$. The direction of the particle, given by the angle θ, change due to coupling to a phoretic field c. The position and orientation of the ith particle is updated (without noise) as $\frac{d\boldsymbol{R}_i}{dt} = \boldsymbol{V}_i$, $\frac{d\boldsymbol{e}_i}{dt} = \boldsymbol{\Omega}_i \times \boldsymbol{e}_i$. Here, the translational velocity $\mathbf{V}_i$ and angular velocity $\boldsymbol{\Omega}_i$ of the ith particle are given as $\boldsymbol{V}_i = v_s\boldsymbol{e}_i + \chi_t \boldsymbol{\mathcal{J}}_i + \mu\boldsymbol{F}_i$, $\boldsymbol{\Omega}_i = \chi_r\left(\boldsymbol{e}_i \times \boldsymbol{\mathcal{J}}_i\right)$. The constants χ_t and χ_r take positive values. $\chi_t > 0$ implies that the particles are repelled from each other, only to be held together by the active chain, while $\chi_r > 0$ implies that the particles rotate away from each other. The force keeping the chain together is modelled as a spring. The force on the ith particle is given as: $\boldsymbol{F}_i = (\boldsymbol{\nabla} U)\big|_{\boldsymbol{r}=\boldsymbol{R}_i}$, where $U = k\left(r_{ij} - r_0\right)^2$ is spring potential of stiffness k and natural length r_0 which holds the chain together. Here $r_{ij} = |\mathbf{R}_i - \mathbf{R}_j|$. We rationalize the results of both experiments and simulations by performing a linear stability analysis on the system.

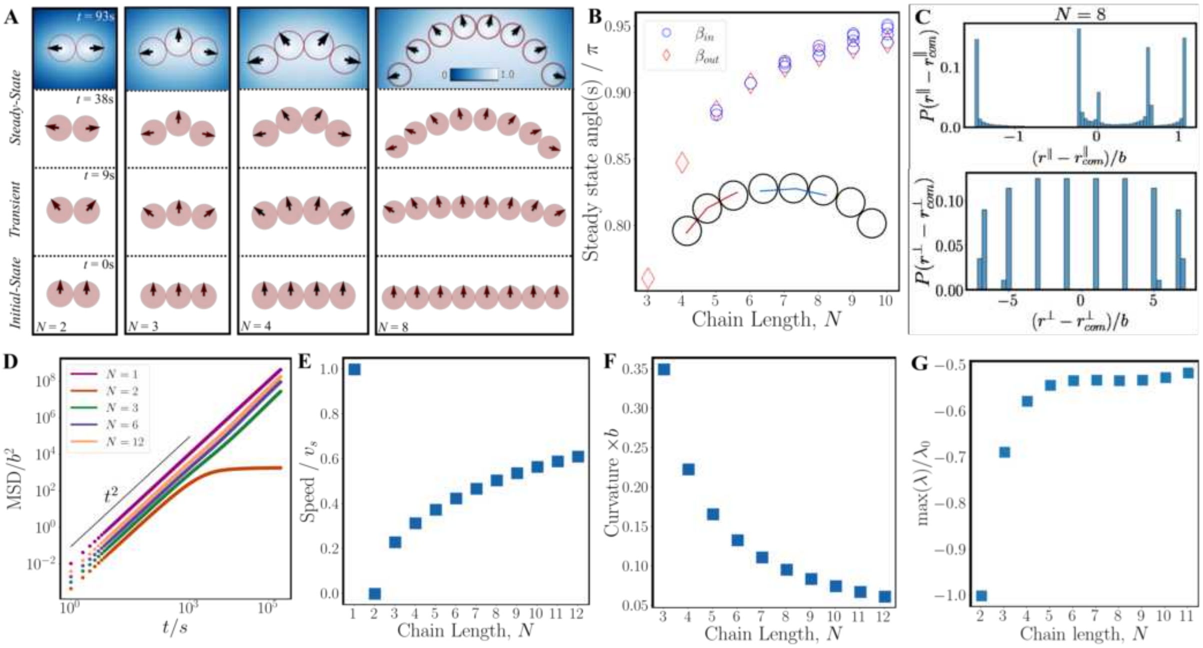

FIG. 1. **Simulations of a minimal model including only chemical interactions capture the active polymer dynamics**. **(A)** Snapshots of active chains from simulations are shown in four columns, for chain sizes of $N = 2$, $N = 3$, $N = 4$ and $N = 8$, respectively (from left to right). Black arrows indicate the orientation $\boldsymbol{e}_i$ of the particles. We show snapshots for the initial-state ($t = 0$), transient-state ($t = 9s$), and steady states ($t = 38s$ and 93s). The pseudo-color plot of the chemical field has also been overlaid on the plots for configuration at $t = 93$s. (**B**) Shows the saturating angles of the chain in the steady state, with β_{in} and β_{out} defined in the inset (visually). Panel(**C**) shows the distribution of monomers on the chain along two directions, corresponding to (from top to bottom) the vertical and horizontal axes in Panel (**A**). Panel (**D**) shows the MSD for different chain lengths, along with the ballistic limit of $\sim t^2$ as reference. Panel (**E**) contains the speed of polymers v^A in steady state, normalised by the speed of a single particle v_s in simulations, as a function of the number of monomers in the polymer (N). The panel (**F**) shows the dimensionless curvature of the active polymer in simulations as a function of the N. Panel (**G**) shows the linear stability analysis of the positional corrdinates, obtained numerically, showing that longer chains are more "rigid" in the sense that the positions of the monomers stabilize the slowest.

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AM - P1

Spontaneous motion of isotropic particles in a Carreau fluid

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The present study numerically investigates the role played by rheology of the suspending medium in altering the self-phoretic dynamics of isotropic active particles. Towards this, a non-Newtonian Carreau fluid is taken as the suspending medium. The analysis shows that a shear thinning fluid significantly reduces the maximum velocity of the particle. The following study uses a finite element based numerical approach to calculate the concentration of the solutal molecules as well as the velocity components of the isotropic particle at finite Peclet numbers. The physical system comprises of an isotropic active particle of radius a which is freely suspended in a non-Newtonian Carreau fluid confined in a microchannel.

Figure 1b shows the variation of the phoretic velocity when the particle is suspended in different shear-thinning fluids with varying Cu. As can be seen from the figure, the critical Peclet number at which the motion of the particle sets in, remains the same (Pe = 4) for all values of Cu. Hence, rheology is seen to have no effect on the critical Peclet number when the particle is suspended in an unbounded medium. On the contrary, the maximum self-propulsion velocity (at Pe = 10) is found to reduce with increase in characteristic strain rate of the fluid (or Cu). However, as Cu→∞, the point of maximum self-propulsive velocity shifts towards a higher value of Peclet number. In addition, the magnitude of the maximum propulsive velocity also increases since the fluid tends to become Newtonian at significantly high Cu.

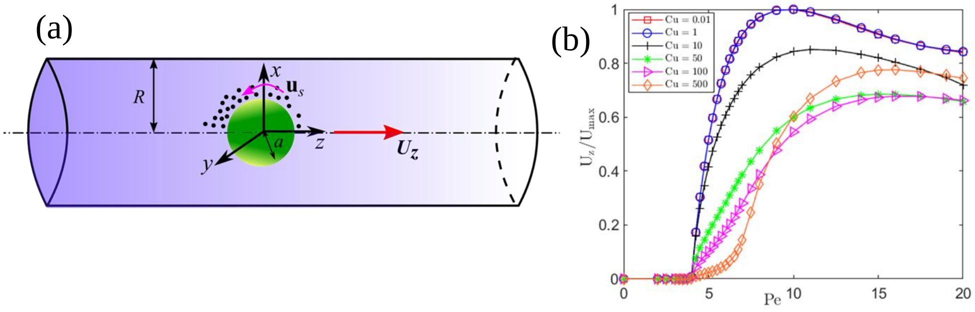

Fig. 1 (a) schematic of the physical system, (b) Variation of normalized axial phoretic velocity of the particle, suspended in a shear thinning Carreau fluid, as a function of Pe.

It can thus be inferred that the rheology does not have a significant effect on the critical Peclet number, at which the propulsion of the particle sets in; however, the maximum velocity as well as the overall variation of the phoretic velocity of the particle with Pe is strongly dependent on the rheology of the fluid.

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AM - P13

Indian Society of Rheology

Dynamics of Nucleating Microdroplets at the Contact Line of Evaporating Multicomponent Drops

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Evaporation of pure and colloidal drops has been studied extensively due to the rich underlying physics and the impact on various applied processes [1, 2]. Much less research has been conducted to explore the fundamental aspects of the evaporation of multicomponent drops [3]. Evaporation drives such systems out of equilibrium, inducing *liquid-liquid phase separation* (LLPS) [4]. Many complex phenomena can occur inside evaporating multicomponent drops, such as Marangoni convection and nucleation of phases. Also, it is known that the nucleated microdroplets at the contact line demonstrate active propulsion by asymmetric interfacial stresses, for example, as in a polyethylene glycol (PEG) and dextran (DEX) binary drop.

In this study, we demonstrate that active microdroplets nucleated near the drop edge move in a stepwise or continuous manner, depending upon their precise location of nucleation. The stepwise dynamics are coupled with random coalescence among microdroplets and the interplay with the gradient of evaporation-driven convective flows. Thus, we show that evaporating multicomponent drops are systems to study the dynamics of active micro-droplets. Our study contributes to the understanding of how micro-swimmers, such as bacteria, in their natural settings.

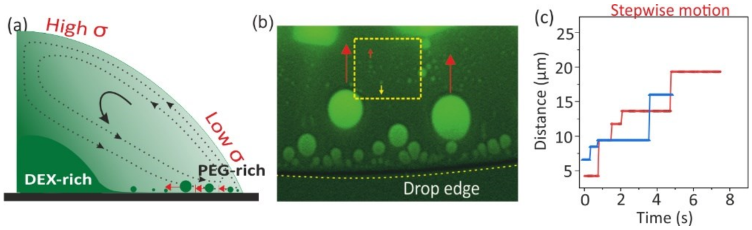

Figure 1: (a) Schematic of Marangoni convection inside an evaporating PEG-DEX drop. Micro-nucleations of DEX are also shown. (b) A zoom-in image of the contact line shows nucleated DEX microdroplets (the big microdroplets are 100 μm in diameter). (c) These microdroplets move towards the bulk of the drop in a stepwise manner induced by coalescence and Marangoni convective flow.

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AM - P48

Flocking by turning away

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The phenomena of flocking, wherein the spontaneous breaking of orientational symmetry leads to emergent collective motion, has been widely studied. Here, we report, combining theory, numerics and experiments on self-propelled metal-dielectric Janus colloids[1], that torques which reorient particle pairs away from each other can exhibit flocking, exhibiting spontaneous alignment of orientations and velocities. Building a coarse-grained description and going beyond mean-field arguments[2,3], we show that an asymmetry in pair distribution function leads the hydrodynamic transport coefficient for the polar order to be non-zero, rendering net non-zero collective torque. Further, using Boltzmann kinetic theory[4], using binary scattering statistics, we show that interactions that turn particles away from each other generically lead to flocking. Our results could help to reconcile the fact that cell trains[5] and layers can flock[6] despite cells turning away from others through contact inhibition of locomotion. Similarly, our work also provides strategies to design robotic collectives that can flock while avoiding collisions by turning away from other robots[7]. More fundamentally, our work shows how macroscopic polar order can emerge even in the absence of microscopic alignment interactions.

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Enhancement in the irreversibility of active processes in viscoelastic bath

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Non-equilibrium active processes are mostly discussed assuming a clear separation of timescales between the system and environment that eventually leads to an effective Markovian description. However, such assumptions will break down if the environment is viscoelastic as the relaxation time of the fluid will be comparatively higher than the viscous media. The effects of viscoelasticity in shaping different active processes are relatively less explored. In this work, with a minimal experiment using a driven colloid in a viscoelastic bath, we show that viscoelasticity significantly increases the mean injected power to the passive object ($\sim 50\%$ compared to a viscous medium), for the same strength of the external driving. Additionally, we observe a notable reduction in negative work fluctuations across a wide range of driving amplitudes. These findings along with an increased rate of entropy production suggest an enhanced irreversibility in driven processes within a viscoelastic bath, which we attribute to the emergence of interactions between the colloid and the viscoelastic medium. We provide a Langevin-based model from which exact analytical results corresponding to the dynamics and fluctuations of the work done in the process are deduced using novel techniques to corroborate all our experimental and numerical findings.

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Indian Society of Rheology

Active Particle Suspensions In Viscoelastic Fluids

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There are many instances in nature where microorganisms migrate in a viscoelastic medium for optimal functionality. For example, motile organisms such as sperm swim in the viscoelastic medium of cervical mucus to fertilize the egg. While it is crucial and fundamental to comprehend the behavior of active suspensions in open systems, most practical systems of interest are under confinement, whether soft or rigid. Recently, Liu et al. observed the self-organization of E. coli bacteria into a rotating vortex that periodically oscillates with a regular frequency, which can be tuned by changing the viscoelasticity of the suspending fluid [1]. This study holds significant importance as it accomplished simultaneous manipulation of the spatial and temporal organization. In this context, we study the dynamics of active particles suspended in a viscoelastic medium of polymer solution under confinement using Dissipative Particle Dynamics (DPD) in two dimensions. In our simulation, the active agents, and solvent are individual DPD particles while the polymer is modeled as a linear chain of DPD particles with Hookean springs between any two DPD particles. The viscoelasticity of the medium is varied by changing the length and concentration of polymer chains. The simulation results are in agreement with the reported findings in the literature, namely at low polymer concentrations the self-organization of active particles within the drop induces rotation of the drop. We present a phase diagram for the drop rotation as a function of strength and packing fraction of active particles at various polymer concentrations.

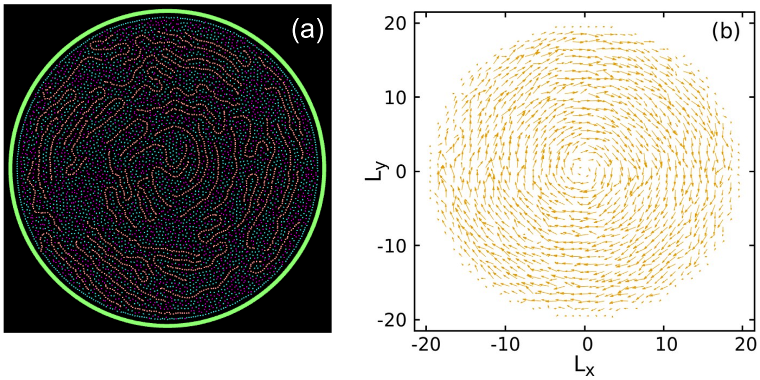

Figure 1:(a) Suspension of active particles in viscoelastic medium of polymer solution under confinement.(b) Corresponding velocity flow field of rotating drop of active particle suspension.

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AM - P4

Interfacial Pusher Bacterium

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Living organisms such as bacteria often form biofilms at fluid-fluid interfaces. In such a scenario, understanding the hydrodynamic interaction between the microswimmer and the interface is quintessential and it is less explored. In this study, we investigate the hydrodynamic flow generated by a neutrally wetted pusher-type microswimmer trapped at a fluid-fluid interface. We use the well-known squirmer model to simulate the flow around the microswimmer. The flow fields are largely affected by the swimming orientation (ϕ) relative to the interface. From the previous study by Gidituri et al. [1], it is known that the steady state orientation of the microswimmer is a strong function of the squirmer parameter (β) and viscosity contrast (λ). The present study explores the flow fields produced by pusher with different orientations. We observe symmetric and asymmetric flows of different strengths depending on the value of β and λ. In order to quantify the flow asymmetry, we defined a parameter called asymmetric index (I). The implication of the generated flow is realized by studying the hydrodynamic interaction between passive tracer particles and the swimmer. We observe that tracer particle trajectories are sensitive to the strength of flow asymmetry.

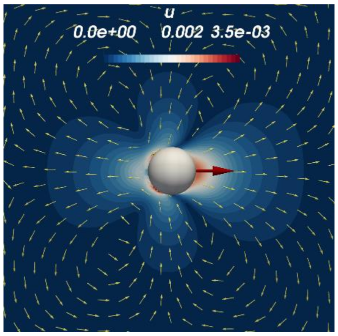

Figure 1: A pusher-type swimmer in the interfacial plane.

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AM - P5

Particle-based mesoscopic model for phase separation in a binary fluid

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We have developed a model to incorporate the phase separation in a binary fluid mixture by augmenting the existing multi-particle collision dynamics (MPCD) [1]. This model features the non-ideal equation of fluid state by considering the excluded-volume interaction between the two components of the fluid mixture. This method is the extension of the work carried out by Ihle et al. In two dimensions [2]. The model can further be extended to study the dynamics of active and passive particles exposed to such systems.

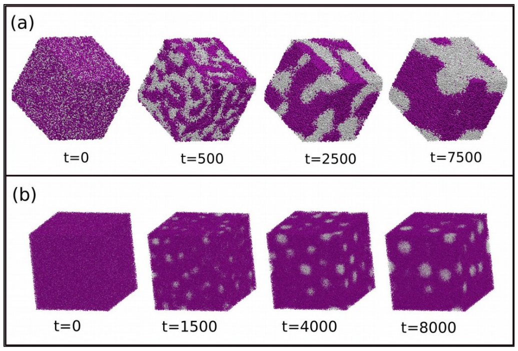

Figure 1: The time evolution of a binary fluid mixture from a mixed phase at time t=0 to a phase separated state at later time. (a) Critical binary mixture (50:50), (b) Off-critical binary mixture (10:90).

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AM - P7

Stochastic migration dynamics of Marangoni surfers between two chambers

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An experimental investigation was conducted, focusing on the migration dynamics of Marangoni surfers between two circular chambers connected by a narrow channel as shown in Fig 1(a). These surfers were generated by punching 6mm diameter disks from A4 size paper and soaking them in a camphor-ethanol solution. The migration dynamics are characterized by Survival probabilities ***S(t)***, (see Fig. 1(b)) of possible configurations which represents the likelihood of a configuration after a time ***t***. In general, the survival probabilities decay exponentially with a characteristic time associated with each configuration. We observe a qualitatively similar behavior among (1) all even-particle experiments and (2) among all odd-particle experiments. For example, in experiments with even number of particles, the most probable configuration is when equal number of particles occupied each chamber. Consequently, fewer migrations of the particles occurred throughout the experiment. Conversely, when there are odd number of particles the most probable configuration is when one chamber has an extra particle than the other. In this state, the extra particle is frustrated and results in lower survival probability for that configuration. Furthermore, we present a simple two-state model to understand and explain the observed dynamics.

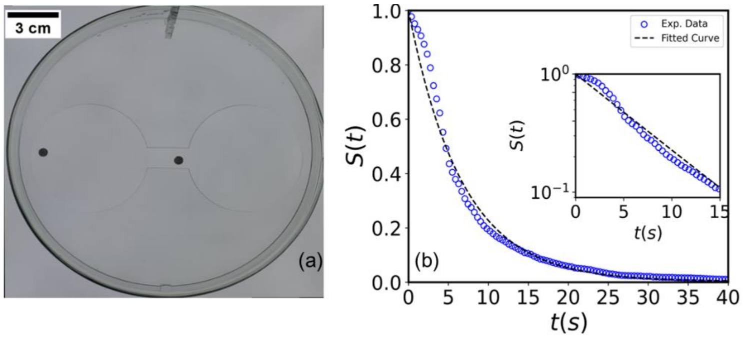

Figure 1:(a). Particles of 6mm diameter inside a dumbbell shaped confinement with each chamber having radius of 3.5 cm connected by a channel length of 2.5 cm and width of 1.2 cm. (b). Survival probability plot for a single particle. Inset: Y-axis plotted on logscale.

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Indian Society of Rheology

Local Polar and Long-Range Isotropic Activity Assisted Swelling and Collapse Dynamics of an Active Ring Polymer

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The circular and ring structures in many synthetic or natural systems simultaneously experience local and long-range forces. In this work [1], we use numerical simulations to investigate the concurrent effect of a local polar and attractive long-range activity on the active ring polymer. While the long-range attraction leads to a systematic collapse, the polar activity [1,2] tends to swell the shorter rings and crumple the larger ones. We show that the steady-state conformation of such an active ring strongly depends on the kind of activity. The dominance of local tangential activity for very short rings, while the long-range activity at intermediate length scales is observed. However, in contrast to our intuition, we observe the dominance of local polar activity again for very large rings. We quantify these observations by comparing the scaling laws and local structures with the passive rings. Further, the relaxation dynamics of the rings show a non-monotonic behavior for polar activity. Such local tangential activity also affects the tumbling and tank-treading motion of ring polymers in shear flow.

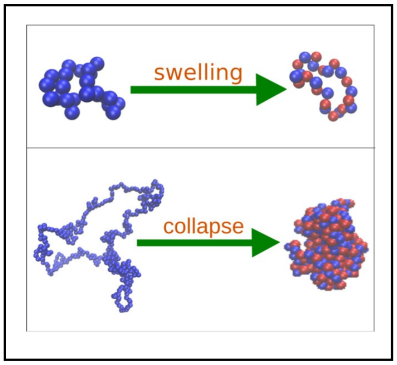

Figure 1: Swelling and collapse of small and large rings respectively.

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Indian Society of Rheology

Collective Dynamics of Active Janus Colloids Using Computer Simulations

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In previous studies, active colloids have brought tremendous attention to researchers for the fundamental study of non-equilibrium systems and their potential applications in pharmaceutical fields [1]. In recent experimental work, Zhang et al.[2] presented the behaviour of metal-dielectric Janus colloids; these are particularly made of silica where half hemisphere is coated with a metallic material. In these colloids, silica and metallic hemispheres polarize differently in the presence of the ac electric field and NaCl solution. The unequal electric polarization on the metal and dielectric hemispheres induce electrokinetic flows that produce self-propulsion[3]. This study highlights the importance of electrostatic torque in clustering phenomena. In contrast to standard Motility-Induced Phase Separation (MIPS), torque-induced aggregation does not require density-induced slowdown. In continuation of the above-mentioned work, another experimental study is done by Linden et al.[4]. The significant finding of this experiment is that (i) firstly, particles aggregate into densely packed clusters, and the size of the cluster rapidly grows, here the effect of excluded volume dominates, and the role of alignment is negligible (ii) and then, The orientational ordering of colloid dominates inside the cluster; as a result, aggregation-fragmentation occurs, and (iii) lastly, the phase separation is interrupted.

Our study explains the fundamental mechanism of these new fundamental phenomena (torque-induced aggregation and interrupted MIPS). We model the Janus colloid at the coarse-grained level and perform 2D Brownian dynamics simulations. A coarse-grained Brownian dynamics simulation approach is employed to study the mechanism underlying various collective phenomena shown by Janus colloids. We model the Janus colloid as a system of two opposite but unequal electric dipoles. We explain torque-induced clustering and interrupted MIPS. The transition from a homogenous gaseous state to aggregated state is studied through cluster analysis. We investigated cluster growth law, probability distribution, and clustering phase in the parameter space of activity and dipolar strength. The dynamics of colloids are described by mean square displacement and density-dependent motility.

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AM - P10

Active droplets dynamics and collective behavior in a capillary

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Biological swimmers exhibit a wide range of dynamic behavior in narrow or restricted spaces and various chemical surroundings. Active droplets serve as an ideal model to gain a deeper understanding of biological organisms by mimicking their activities in inanimate systems.[1] Here, we report the individual and collective behavior of oil droplets in a capillary channel filled with aqueous solutions, whose self-propulsion is caused by micelle solubilization.[2] In the presence of high macromolecular solute (polyethylene oxide, PEO) or molecular solute (glycerol) in trimethyl tetradecyl ammonium bromide (TTAB) solution, droplets avoid contact with the boundaries and, in TTAB, undulate in the channel or propagate linearly along the capillary wall. For the interaction of collective droplets, upon injection of multiple droplets in the glycerol-TTAB solution from one end of the capillary, a secondary droplet chases the leader, resulting in trailing-like behavior. In TTAB solution, chasing becomes metastable and in polymer-TTAB solution, repulsive interactions between droplets lead to their separation. When droplets are injected from both ends of the channel, dispersion-like behavior occurs upon contact or close proximity. Moreover, their interactions in PEO induce spherical symmetry breaking. Droplets' motion and collective interactions in the confined geometry are explained by characterizing the chemical and hydrodynamic flow field near the locality of droplets. This study unveils the hitherto unexplored collective motion and deformation of active droplets in a capillary.

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AM - P11

Indian Society of Rheology

Active Droplets in Gravity

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Active droplets or micro-swimmers, which can move autonomously through a fluid medium without any external forcing, inevitably encounter external force or flow field [1-2]. While the self-propulsion motion of active droplets and particles has been explored extensively, the motion in the presence of an external force is not well understood. To this end, we investigate the motion of an active droplet subjected to gravitational force through a combination of theory and numerical simulations. A significant amplification in the droplet velocity is observed as one increases the strength of advection relative to the diffusion (through the dimensionless parameter Péclet number (*Pe*). In the theory, matched asymptotic methods are employed to obtain both global and local solutions which are also compared successfully with the finite element-based numerical simulations. We have demonstrated some specific examples where the droplet can move against the direction of the external force. The mobility contrast between the two phases turns out to be crucial in altering the droplet dynamics. We believe that the present findings will lead to a comprehensive understanding of how active droplets behave in real-world environments or in practical scenarios, where an external force or an external flow field is typically present. Furthermore, the framework given here will be useful in carrying out experiments involving active droplets or emulsions by providing a concrete concept about the involved parameters, allowing them to be optimally tuned to achieve desired functionality.

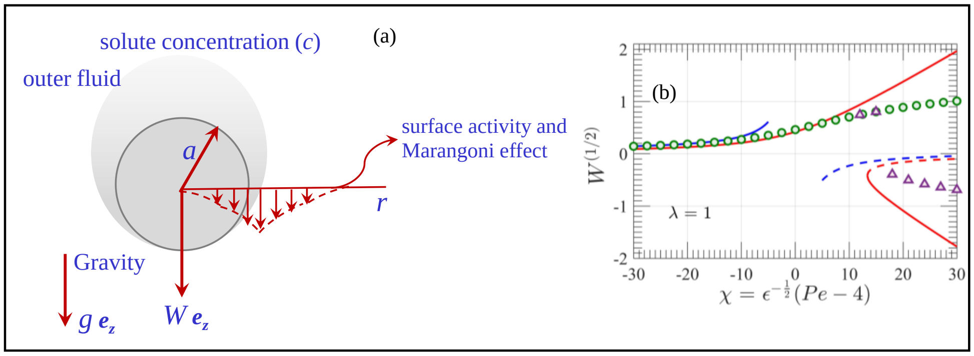

Figure 1: (a) Schematic of an active droplet in the presence of gravity. (b) Droplet velocity as a function of χ based on global (blue lines) and local (red lines) analysis.

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AM - P12

Characteristic features of self-avoiding active Brownian polymers under linear shear flow

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We present Brownian dynamics simulation results of a self-avoiding flexible polymer chain under linear shear flow in the presence of active noise. The active noise strongly affects the polymer conformational and dynamical properties under shear flow, such as the stretching in flow direction and compression in the gradient direction, shear-induced-alignment, and shear viscosity, and in the asymptotic limit of large activities and shear rates, their power-law scaling exponents differ significantly from that of passive chains. The chain's flow-induced stretching at a given shear rate is reduced by active noise, and it displays a non-monotonic behavior, where initial chain compression is followed by its stretching with increasing active force. The compression of the active chain in the gradient direction follows the relation $\sim Wi_{Pe}^{-2/3}$ as a function of the activity-dependent Weissenberg number Wi_{Pe}, which differs from the scaling observed in passive systems $\sim Wi_{Pe}^{-1/2}$[2]. The flow-induced alignment at large shear rates $Pe >> 1$, where Pe is the P'eclet number, and large $Wi_{Pe} << 1$, displays the scaling behavior $Wi_{Pe}^{-1/3}$, with an exponent differing from the passive value $1/2$. Furthermore, the polymer's zero-shear viscosity displays a non-monotonic behavior, decreasing in an intermediate activity regime and increasing again for large Pe induced by excluded-volume interactions. The shear viscosity is found to decrease with the Weissenberg number following the power-law relation $Wi_{Pe}^{-\beta}$, where $\beta = 1/2$[3,4] and $\beta = 2/3$ for passive and active polymers, respectively. In addition, our simulation results are compared with the results of an analytical $model$[1], which predicts quantitively similar behaviors for the various aforementioned physical quantities.

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AM - P14

Light-activated rod-shaped colloidal microswimmers for exhibiting multimode dynamics

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Manipulating and tuning the rich dynamics in the active colloidal systems has been a key motivation in the last few years for understanding the naturally occurring active matter systems and play a crucial role in creating advanced functional materials for harnessing in micro/nanorobotics.[1] With this motivation, we have fabricated rod-shaped particles and demonstrated their swimming behavior by energizing them with the externally supplied light source. The rod-shaped swimmers were fabricated by taking advantage of both Langmuir-Blodgett (LB) method and e-beam assisted Glancing angle deposition (GLAD) technique. [2,3] Following the above deposition route, we have successfully created three rod-like particles named as pristine titania rod, hybrid-1, and hybrid-2 structures. All these structures contain 1 µm silica microsphere head at its bottom, and on top of it, the elongated arms were grown using two different photocatalytic materials (TiO_2/Cu_2O). While forming the components of these rods, we have carefully implanted the active catalytic materials at particular sites to induce a specific type of motion by responding to either UV or Visible light. The pristine titania rod showed the linear forward motion upon switching the UV light. Further, the dynamics of the hybrid-1 structures were illustrated, and it was found that they exhibited axial rotation in Visible light and helical motion in the UV region. On the contrary, the hybrid-2 rods were programmed to show linear motion in Visible and helical motion upon the irradiation of the UV light source. Numerical simulations were performed for all structures using COMSOL Multiphysics software, which depicted a good agreement with the experimental findings. We anticipate that our facile fabrication routes would promote synthesizing some more different complex structures to explore other intricating dynamical phenomena and bring a tremendous possibility in applying such swimmers in micro/nanorobotics for targeting numerous applications such as cargo delivery, fluid mixing, sensing, etc. in the lab-on-a-chip or microfluidic devices.

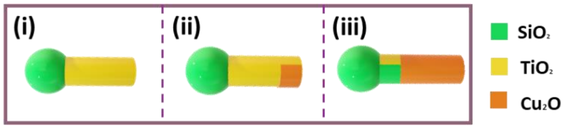

Figure 1: Schematics of rod-shaped colloidal microswimmers. (i) pristine titania rod, (ii) hybrid-1 rod, and (iii) hybrid-2 rod.

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Self-propulsion behaviour of cubic shape Janus particles: Effect of shape anisotropy on longer range ballistic motion

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Self-propulsion is the ability of an object or organism to generate the energy required for its own movement, independent of external forces. In nature, organisms like bacteria show such behaviour by converting chemical energy to mechanical motion [1]. Inspired by this, the motion behaviour of artificial particles like Janus particles has been widely studied. However, most of the works are on isotropic particles such as spherical shape; there are very few literatures where anisotropic particle like cube shape particle has been studied [2][3]. In this work, a cube-shaped platinum-coated hematite Janus particle (HM-Pt) of approximately 883 nm has been used to study the self-propulsion behaviour, using hydrogen peroxide (H_2O_2) as a fuel medium. In regard to study the shape effect, the self-propulsion trajectories of spherical shape half platinum coated polystyrene (PS-Pt) and HM-Pt Janus particles have been compared. It has been observed that the PS-Pt particles show enhanced Brownian behaviour over a longer time scale, while the HM-Pt particle has ballistic or directed movement. As polystyrene is a non-conductive material, it only shows a self-diffusiophoresis mechanism in H_2O_2 solution, while hematite is a semiconductor in nature, it can show both self-diffusiophoresis in H_2O_2 solution and self-electrophoresis mechanisms of self-propulsion under UV light in H_2O_2 solution. Therefore, further study on the self-propulsion behaviour of HM-Pt particles under varying UV-light intensity has been analyzed. Due to the self-electrophoretic mechanism, the velocity of the particle increases under UV light intensity. It can be imputed to an increment in the catalytic activity of the particles, which produces O_2 molecules and H^+ ions due to the decomposition of H_2O_2. This creates an asymmetric electric field, leading to enhanced electroosmotic flow around the particles; correspondingly, particles cover more distance in the same time scale.

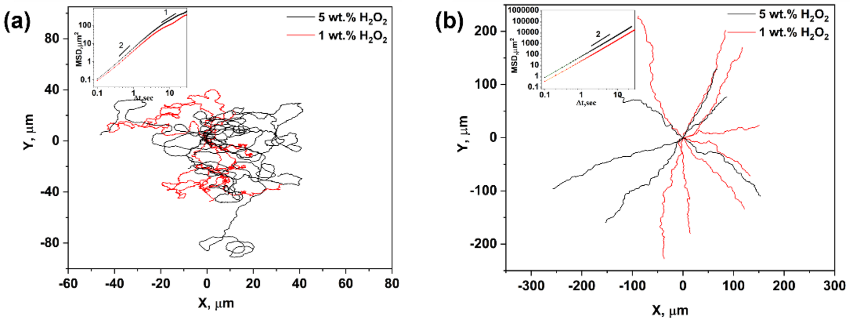

Fig 1: (a) Trajectories of PS-Pt particles and (b) HM-Pt particles in 1 and 5 wt.% H_2O_2, also their respective MSD vs. Δt plots inserted, (1wt.% red color and 5 wt.% black color).

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Indian Society of Rheology

Tumbling dynamics of an active filament in simple shear flow

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Many biological filaments, such as cytoskeletal filaments of the cells, flagella and cilia of bacteria etc. are made of composite active elements such as molecular motors moving on passive filaments. In a fluid medium, these elements can act either as extensile or contractile force dipoles resulting in self-propulsion [2,3]. The interactions between these active filaments and fluid flows are ubiquitous and essential in many biological processes in nature.

Herein, we use a modified overdamped Langevin equation to study the dynamics of an extensile active filament in simple shear flow. The active filament is modeled as a chain of active beads connected by potentials that enforce inextensibility, semi-flexibility, and self-avoidance. To capture the motion of extensile filaments in a fluid medium, the active element on each bead is modeled as a force proportional to the local curvature of the filament. The effect of activity and shear rate on the dynamics of tumbling is studied for filaments of different lengths and bending stiffness. We see three distinct regimes in the tumbling interval as a function of shear rate, with a shear rate independent regime sandwiched by an activity-dominated regime and a shear rate-dominated regime. The tumbling interval is smaller than that of the passive filament for the low shear rates and larger for the high shear rates, with the crossing over in the shear rate independent regime. At high shear rates, the active filament follows the same power law for the tumbling interval as that of the passive filament. The strength of the activity increases the shear rate required to reach this scaling regime while increasing length decreases it. Our results can be useful for a better understanding of the rheology of soft active materials.

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Self-propelled microrobot for pH sensing applications

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Microscale robots, or microrobots, have gained significant attention in recent years due to their potential applications in various fields, including healthcare, environmental monitoring, and industrial automation [1,2]. One crucial aspect of microrobots is their ability to perform specific tasks autonomously in complex environments. The development of a microrobot pH sensor is motivated by the need for precise and real-time pH measurements in localized areas, particularly in biological systems and industrial processes. Traditional pH sensing methods often rely on bulky equipment or large-scale probes, limiting their applicability in microenvironments. By leveraging advancements in microfabrication and sensing technologies, we present a miniaturized microrobot with integrated pH sensing capabilities. The microrobots are Janus-shaped particles having a coating of the photocatalytic active layer (Copper oxide or titanium dioxide) over the photo-catalytically inert silica microsphere. These microrobots exhibit autonomous propulsion by exploiting the fuel medium (hydrogen peroxide) under the irradiation of matching band gaps of external light energy [3]. Additionally, a magnetic layer is coated before the photocatalytic layer for the directional swimming of microrobots. Thereafter, the microrobots were modified with a sequential tagging of a pH-responsive fluorescent dye through a physical vapor deposition technique. The fluorescent signal intensity changes according to the pH of the medium due to the change in the molecular structure of the dye. Therefore, the multicomponent-designed microrobots are capable of active guided swimming to reach the source site for measuring the local pH change on demand. The miniaturized form factor, autonomous capabilities, and high-precision pH measurements make the microrobots a promising tool for various applications, including biomedical research, environmental monitoring, and quality control in industrial processes.

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AM - P20

Nematic Droplets in Structured Optical Field

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Nematic liquid crystals have both fluid like and crystalline properties due to their anisotropic molecular alignment .When confined these in the form of droplet, these nematic liquid crystals exhibit defects and topological structures.

Nematic droplets are sensitive to change in external factors like optical field, electric field, temperature and concentration. An effective way to understand interaction between optical fields and droplets is to use optical tweezers. This allows us to investigate and manipulate their behavior in a confined and controlled environment. The inability of conventional optical tweezers to give multiple dynamic traps of nematic liquid crystal droplets in three dimensions with high level of accuracy has led us to use structured optical traps. Structured light has emerged as an important tool to interrogate and manipulate confined soft matter systems [1, 2]. One form of structured optical field is holographic optical tweezers which provides precise control over trapping potentials, enabling the creation of custom shaped confinement geometries.

In this work, the optical forces due to holographic optical tweezers are harnessed to study non equilibrium dynamics and assemblies of nematic droplets. The trapped nematic droplets, under certain controlled conditions, exhibit intriguing topological structure revealing the interaction between droplet interfaces and defects. Through real time imaging we explore the translational and rotational dynamics of trapped liquid crystal droplets.

In conclusion, these investigations on nematic droplets in the structured optical field offer valuable insights into the interplay between confinement, topology and orientation dynamics with potential applications in topological optics and in soft optical devices.

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Effect of real-space circulating currents on the bubble phase separation of active particles

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Active matter (AM) is an inherently non-equilibrium system that consumes energy from the surroundings to perform the work. Such systems lack time-reversal symmetry, resulting in the violation of detailed-balanced conditions. The scale of active units in nature ranges from the cytoskeleton of eukaryotic cells to whole bacterial colonies, bird flocks, schools of fish, herds of sheep, and even humans [1, 2]. Such a system's non-equilibrium nature reveals many intriguing behaviors such as collective motion, giant number fluctuation, breaking of rotational symmetry in two-dimension, etc. To understand the non-equilibrium phenomenon of domain growth in spherical polar active particles, we use scalar active model B+ (AMB+) [3, 4]. This model includes terms that arise from the actions leading to non-equilibrium currents, characterized by both zero and non-zero curl, in a steady-state. These terms are not permissible within the framework of equilibrium models applied to passive particles. The impact of non-zero curl currents on phase separation is investigated with critical composition.

Our extensive numerical simulations demonstrate the decrease in the domain growth due to the activity responsible for rotational current. In the equilibrium scenario, where particles are passive, the growth exponent for phase separation is denoted as $L(t)=t^a$, and $a=1/3$ [5]. Intriguingly, the introduction of activity leads to a slow down in growth dynamics, as signified by the exponent exponent $a=1/4$. Another significant result of our study is the revelation of freezing behavior when both active and passive currents are in competition. The mean size of the domains shows scaling behavior with respect to the activity of the system.

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AM - P22

Indian Society of Rheology

Phase Transition In Active Nematics

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Motivated by recent experiments on rod-like particles [1], in our case significant attention has been devoted to conducting numerical simulations that explore the active behavior of apolar rods in a confined two-dimensional system subjected to vertical vibration in the third direction. These apolar rods form a nematically aligned system above a threshold rod concentration. The threshold concentration decreases with the rod length. While the ordered phase lacks long-range positional order, it exhibits a global orientational order.

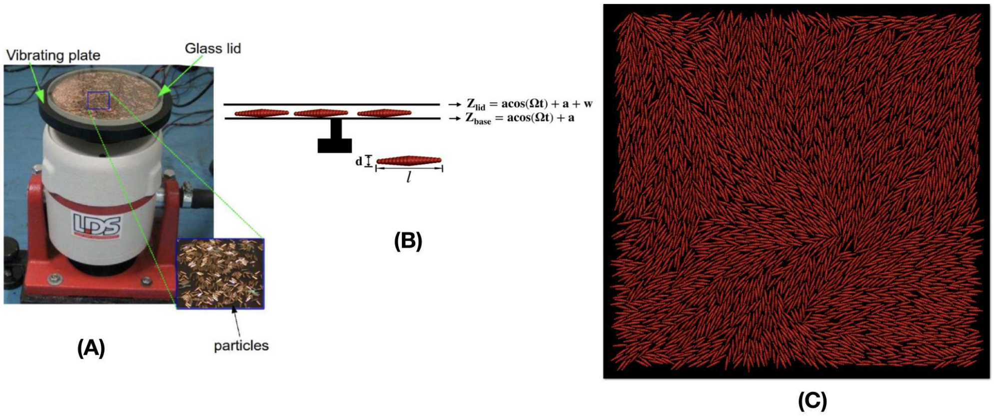

Figure: **(A)** An experimental setup for vertically shaken monolayer (Nitin Kumar, A K Sood Lab), **(B)** Schematic diagram of the vibrated granular nematic system, **(C)** Screenshot of the system.

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AM - P23

RODROLLS: Self Rolling Rods powered by Light and Chemical gradients

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The self-rolling motion upon spontaneous symmetry breaking is demonstrated by certain rod-shaped microorganisms like viruses [1][2]. Hence it is imperative that we understand the mechanism of this symmetry breaking triggering the active rolling motion. It is very interesting to try and replicate this on a microscopic scale. The main aim of the project is to create a new class of active rods that exhibit rolling activity under chemical and optical gradients. To achieve this, it is important to understand the mechanism of activity of rod-like objects under chemical and optical stimuli.

Experiments conducted using silica Janus rods with a Platinum layer in an aqueous solution of H_2O_2 give interesting results and exhibit different kinds of activity when parameters like concentration of H_2O_2 and aspect ratio of rods are changed. Under specific conditions, particles are capable of switching their direction of motion. Studying these rods under chemical and optical gradient shows promising results.

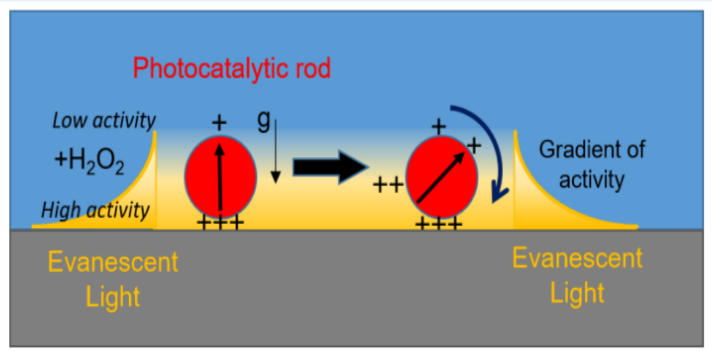

Figure 1: schematic of an active rod in light and chemical gradient.

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AM - P24

Pair and Collective Dynamics of Active SiO_2-Pt Active Janus Colloids

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Janus colloids can perform self-propelled motion under the influence of a self-generated physical/chemical gradient. Our study attempts to understand the collective dynamics of self-diffusiophoretic SiO_2-Pt Active Janus Colloids (AJCs). We first set out to understand the collision dynamics of isolated AJC pairs. We classify these 'collisions' based on the AJCs' orientations before and after their physical contact. The interplay of hydrodynamic and chemophoretic interactions leads to a noticeable decrease in the particles' speed with complicated orientation changes. These changes and the time of physical contact are significantly influenced by the initial approaching speeds and orientations of the particles. As the particle concentration within the system increases, the frequency of interparticle interactions (pair-interactions and more) rises, resulting in reduced average speeds and reorientation timescales of the particles. Notably, at intermediate particle concentrations, dynamic clustering phenomena are also observed. Our study provides useful insights into the collective dynamics of active Janus Colloids and enhances our understanding further of their applicability in various futuristic technologies.

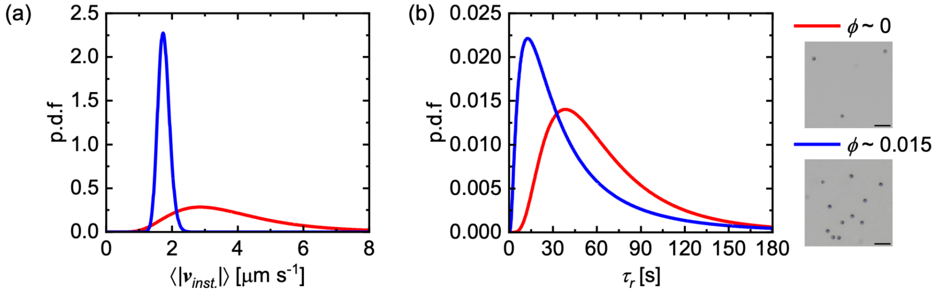

Figure 1: Fitted log-normal probability distribution function curves of (a) the average instantaneous speed $\langle|\boldsymbol{v}_{\mathrm{inst.}}|\rangle$ and (b) reorientation timescale $\boldsymbol{\tau}_{\mathrm{r}}$ for systems with two different particle area fractions $\boldsymbol{\phi}$. As $\boldsymbol{\phi}$ increases, the distribution narrows and the peak shifts to the left. The scale bars in the optical micrograph correspond to a 25 $\boldsymbol{\mu}$m length.

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Enhanced Activity Reduces the Duration of Intermittent Lévy Walks in Bacterial Turbulence

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Dense bacterial suspensions display collective motion exhibiting coherent flow structures reminiscent of turbulent flows. In contrast to inertial turbulence, understanding the microscopic dynamics of bacterial fluid elements undergoing collective motion is in its incipient stages. Here, we report experiments revealing correlations between the microscopic dynamics and the emergence of collective motion in bacterial suspensions [1]. Our detailed analysis of the passive tracers and the velocity field of the bacterial suspensions allowed us to systematically correlate the Lagrangian and the Eulerian perspectives. Bacteria within the collective dynamics revealed initial ballistic dynamics followed by intermittent Lévy walk before the eventual decay to random Gaussian fluctuations. Intriguingly, the persistence length and time of the fluid motion decrease with an increase in the activity, which, in turn, reduces the duration of Lévy walk. Our results reveal transitions in microscopic dynamics underlying the bacterial turbulence and their control via the intrinsic time scales set by the effective activity of the flow.

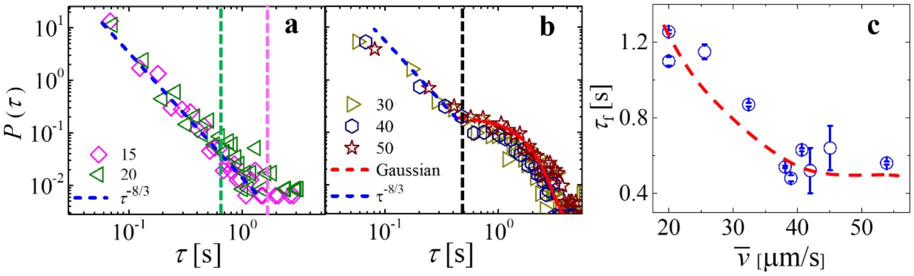

Figure 1: (a, b) Probability distribution of waiting time (τ) for different bacterial concentrations in the units of c/c_0 ($c_0 \approx 10^8$cells/mL): (a) For less concentration (i.e., $15c_0$ and $20c_0$), distribution shows a power law like behavior with $\tau^{-8/3}$ scaling. (b) For higher concentrations (i.e., $c > 20c_0$), the distribution shows a Gaussian tail after a particular time scale. (c) Flow correlation time as a function of effective activity (mean velocity) of the suspension (dashed line is a guide to the eye).

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Indian Society of Rheology

Universal scaling underlying the evolution of bacterial interfaces: A case study on swimmers vs. non-swimmers

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Convective flows during the evaporation of suspensions drag the particles to the pinned interface leading to their enrichment at the edge of the droplet. The statistical properties of the evolving interface at the pinned edge are often characterized by its mean height ($\bar{h}(t)$) and its standard deviation ($w(L,t)$). The time and length scale dependence of these quantities reveal power laws: $w(t) \sim t^{\beta}$ and $w(L) \sim L^{\alpha}$. Here α and β respectively characterize the roughness and the growth of the interface and, in turn, the type of universality classes [1]. Here, we explore the statistical properties of the evolving interfaces obtained by the evaporation of suspensions of living bacteria. We performed systematic experiments on swimming and non-swimming bacteria of different aspect ratios, which allowed us to delineate the role of aspect ratio and active swimming on the spatiotemporal evolution of interfaces. With increase in the aspect ratio, the non-swimming bacteria exhibit a transition from $\beta = 0.5$ (for spherical bacteria) to $\beta = 0.7$ (for long rods), suggesting kinetic roughening for longer rods. This is in accordance with the observations on passive colloids of different aspect ratios [2]. However, in contrast to the passive particles, long rod-like swimming bacteria smoothen the interface over time leading to $\beta = 0.35$. Intriguingly, the roughness exponent $\alpha = 0.5$ is constant for all the systems. While the swimming ability and the aspect ratio control the kinetic roughening, all bacterial interfaces exhibit Kardar Parisi Zhang-like scaling [1,2]. Thus, in comparison to the passive interfaces, our results reveal interesting deviations in the interface evolution of living bacterial interfaces. We believe that a detailed understanding of such evolving bacterial interfaces may allow us to understand the physics underlying the expansion of bacterial communities like swarming colonies and biofilms.

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Indian Society of Rheology

Dynamics of Bacterial Swarming on a Solid Porous Media

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In this study, we employ a comprehensive two-phase model to analyze the dynamics of bacterial swarming on porous substrates. The two distinct phases under consideration are the cell and aqueous phases. We use the thin-film approximation, as the characteristic height is significantly lower than the radius of the swarm colony. Through numerical simulations, we predict the swarm height, the volume fraction of each phase, and the profiles of surfactants within the swarming colony. Notably, we account for the impact of osmotic flow on the dynamic behaviors exhibited within the swarm. Additionally, we include the slip condition to account for the wettability of the substrate. Our model shows that the increase in the wettability of the substrate leads to faster expansion, while increased surface tension forces redistribute biomass radially.

Our framework accounts for the interaction between mechanical stress from bacterial migration and Marangoni effects. Our mathematical model helps explain instability in bacterial colony pattern. We compare our model predictions of osmotic influx with experimental data from previous studies [1].

Keywords: Bacterial swarm, Thin-film approximation, Marangoni effect, Front instability.

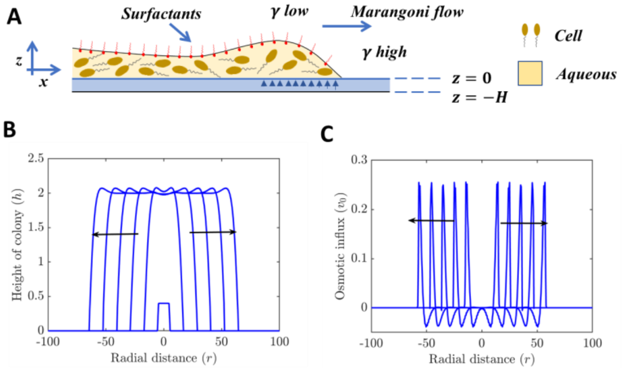

Figure 1: **A)** Schematic of a bacterial swarming on a substrate covered by an insoluble surfactant. The schematic of two phases is represented on the right-hand side. **B)** Numerically obtained height of swarm (h). **C)** Variation of the osmotic influx (v_0) within the colony. The solution profiles are plotted in an increment of $t = 10$.

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Soft makes it hard to swim: Role of microconfinement elasticity in active swimmer dynamics

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Self-propelled droplet microswimmers or active droplets [1-3], driven by micellar solubilization, provide a simple biomimetic model system for studying the response of biological micro-swimmers to external stimuli by circumventing biological complexity. Here, we investigate the role of elastohydrodynamic cues in altering the swimming dynamics of self-propelled active droplets in microconfinements (Fig. 1(a)) of varying softness (elasticity). We observe that active droplets swimming near a wall in a softer micro-confinement (higher El) exhibit lower, and gradually decreasing, instantaneous self-propulsion velocity compared to those in a rigid one (compare Figs. 1(b) and (c)). In a softer microchannel (Fig. 1(d)), the active droplet not only exhibits lower velocity, but also frequent reorientation events indicating a loss of directionality (compare Figs. 1(e) and (f)). Finally, we probe the role of wall elasticity in such alterations in the dynamics of active swimmers in microconfinements by combining elements of Stoksean flows and elastohydrodynamics.

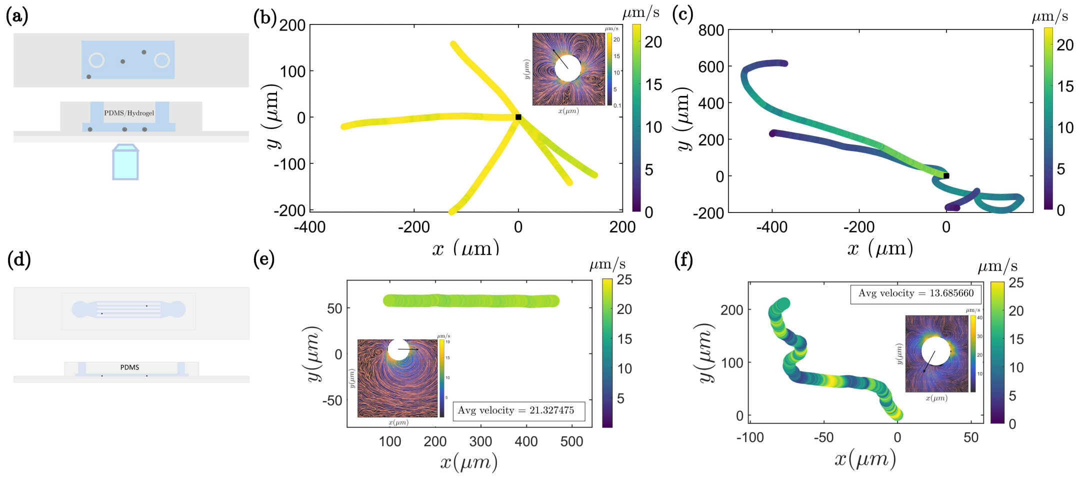

Figure 1: (a) Schematic of the strong micro-confinement ~80μm in height. (b, c) Swimming trajectories color coded with instantaneous velocities of the self-propelled droplet microswimmers in micro-confinement with quiescent medium having elastoviscous number ($El = \mu U_0/ER$), $El = 2.75 \times 10^{-9}$ and $El = 2.77 \times 10^{-8}$ respectively; (fig.1(b)inset) strong pusher flow field. (d) Schematic of the channels ~160μm in width, ~80μm in height). (e, f) Swimming trajectories of active droplets in microchannels having $El = 2.75 \times 10^{-9}$ and $El = 1.44 \times 10^{-8}$ respectively; (fig.1(f)inset) shows the flow field.

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AM - P31

Dynamics of an active Belousov-Zhabotinsky droplet in shear flow

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Active droplets, powered by internalized chemical reaction, that are capable of exhibiting directed motion in a background flow, are perfect candidates for designing biomimetic systems. Apart from biological systems, active droplets have significant applications in emulsion processing, microfluidic technologies, biological cell systems, and so on. In this work, we investigate the dynamics of an active droplet driven by the oscillatory Belousov-Zhabotinsky (BZ) reaction in a confined shear flow, using the lattice Boltzmann method in conjunction with phase-field model. Our work provides insights into the combined effect of reaction kinetics, droplet deformation and the strength of confined fluid flow on the dynamics of the active droplet. We illustrate that the background shear flow leads to the formation of concentration nucleation spots in the droplet, which generates asymmetric gradients in the interfacial tension, thereby driving the droplet via the Marangoni effect in a particular direction. Furthermore, we demonstrate that the location of nucleation spots and therefore, the droplet trajectories can be controlled by the nature of surfactant, the strength of flow field and BZ reaction kinetics. Thus, in contrast to a passive droplet in a shear flow that only migrates towards the wall, an active droplet exhibits a spectrum of behaviours as shown in Fig. 1. In essence, our study unveils the fascinating interplay of background flow and self-propulsion, thus unfolding the underlying mechanism for the directional motion of an active BZ droplet. We believe that our findings not only provide a mechanism to control the motion of chemically-driven active droplets but also open up avenues to harness these design rules for a variety of microfluidic and biophysical applications.

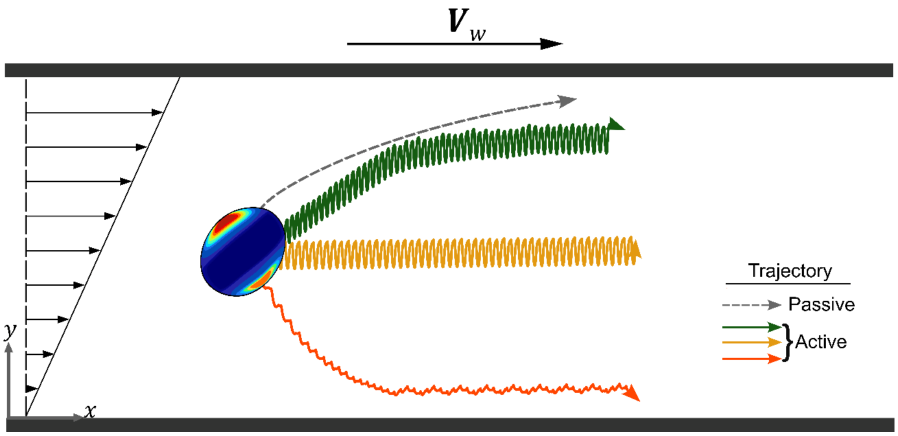

Figure 1: Schematic representation of an active BZ droplet in a shear flow

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AM - P32

Dynamics of the asymmetrical self propelled particle in a ordered crowded environment

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The presence of active particles is ubiquitous in the biological environment which follows nonequilibrium laws. Biological systems are inherently crowded with packing fraction upto 40%. The study of passive tracer particle in ordered crowding is extensively studied, however the dynamics of active particle does not get its due attention. In particular, we study the diffusive dynamics of the janus particle in a continuum space available between periodic lattice points that acts as crowders. We investigated the effect of crowder attraction on the janus particle as well as the interplay between the inherent property of self propulsion and the adsorption due to attraction. We carried out the translational and rotational mean square displacement calculation, diffusion coefficient to inquire diffusive properties and van hove correlation function to observe the trapping properties due to the obstacles. We noticed that the translational and rotational decoupling happening at intermediate time with varying packing fraction and couples at higher packing fraction. The van hove correlation function also peaks as self propulsion increases. Indeed, this computational study will help to manufacture many artificial active agents which can help in efficient drug delivery.

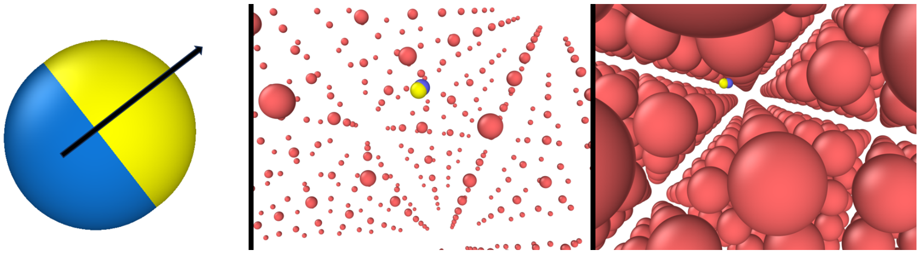

Figure 1: Schematic representation of the janus particle (left). The schematic represents the janus particle inside obstacles of varying packing fraction with lower ϕ (middle) and higher ϕ (right).

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AM - P33

Coarsening arrest by active-rotor turbulence in a binary-fluid system[*]

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We use a generalised Cahn-Hilliard-Navier-Stokes(CHNS) model, with one scalar order parameter ϕ coupled to the velocity field, to study active-rotor turbulence in a two-dimensional (2D) binary-fluid system with friction. In our direct numerical simulation (DNS), we solve these generalised CHNS equations by using a pseudospectral method to study active-rotor turbulence, which arises because of gradients in the concentrations of clockwise- and anticlockwise-rotating particles. We obtain various statistical properties of this turbulence, e.g., the energy spectrum, energy flux, and the Okubo-Weiss field, and we show that it suppresses phase separation [like conventional fluid turbulence does].

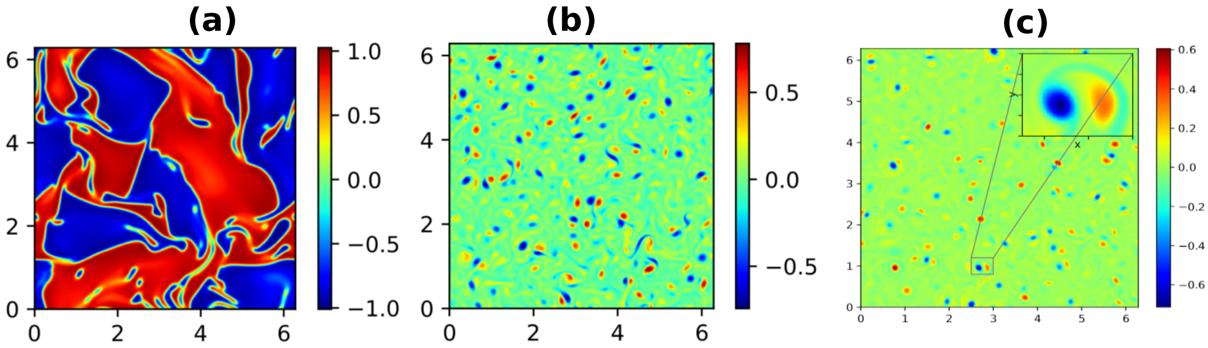

FIG. 1. Illustrative pseudocolor plots of ϕ with the activity τ(increasing from left to right) for (a) $\tau = 0.5$ (showing the passive phase-transition) , (b) $\tau = 4.0$ (showing the large size of doublets) , and (c)$\tau = 15.0$ (showing the small size doublets) ; the phase separation is suppressed with increasing the activity (τ).

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[*] A footnote to the article title

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Motility Induced Phase Separation in Quorum Sensing Particles

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Quorum Sensing is an inter-cellular communication mechanism commonly used by bacteria, and this typically involves the release and detection of chemicals known as Auto-Inducers (AIs) [1]. An interesting phenomenon seen in active matter is the ability of particles to spontaneously separate into dense and dilute phases, because of alterations in their motility, either due to physical interactions, chemical interactions or a combination of both [2]. It is known that AIs can repress the motility of a cell by gene-regulatory mechanisms, in the LuxIR network [3], for example. However, very little is known about the role of Quorum Sensing on the collective dynamics and self-organization of these active particles. Here we employ Brownian Dynamics (BD) simulations to show that Quorum Sensing can lead to phase separation, when the motility response of particles, to change in chemical concentration is high enough. We make quantitative predictions on the existence of a phase separated state and verify these predictions with a continuum model. This not only verifies the claims from our numerical simulations, but also helps us identify fundamental mechanisms behind the occurrence of phase transition. We envisage that the present research will further our understanding on how sub-cellular processes can lead to emergent patterns at the population level.

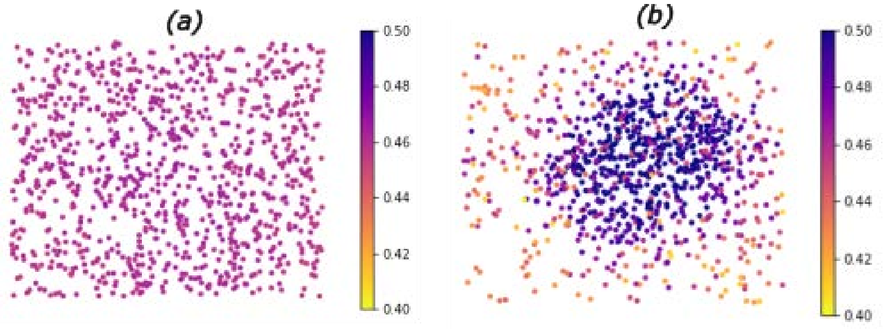

Figure 1: Steady state configuration of motile particles, obtained from BD simulations for (a) low motility response and (b) high motility response. The color denotes the value of an intracellular chemical which is responsible for Quorum Sensing. The key observation here is the fact that a high motility response (b) leads to phase separation.

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Indian Society of Rheology

When does an active bath behave as an equilibrium one?

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Abstract

Active baths are characterized by a non-Gaussian velocity distribution and a quadratic dependence with active velocity v_0 of the kinetic temperature and diffusion coefficient. While these results hold in over-damped active systems, inertial effects lead to normal velocity distributions, with kinetic temperature and diffusion coefficient increasing as $\sim v_0^{\alpha}$ with $1 < \alpha < 2$. Remarkably, the late-time diffusivity and mobility decrease with mass. Moreover, we show that the equilibrium Einstein relation is asymptotically recovered with inertia. In summary, the inertial mass restores an equilibrium-like behavior.

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Spontaneous flow transition of active nematics in a wavy walled channel

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The confinement of a dense suspension of active nematics within channels has been shown to lead to spontaneous flow transitions beyond a critical activity, resulting in the emergence of distinct flow states [1,2]. Recent experiments involving a mixture of microtubules and clusters of kinesin motors, constrained within a toroidal geometry featuring exterior ratchets, have demonstrated that the spontaneous flows can be tuned to a specific direction [3]. Motivated by these experimental observations, we analytically and numerically investigate the effect of wavy walled channels on the underlying hydrodynamics of active nematics.

Using multiparticle collision dynamics algorithms developed for simulating active nematics [4] we demonstrate the spontaneous flow transition in flat and wavy walled channels. In the former case, the numerical simulations are in accordance with the scalings predicted by the linear stability analysis. In case of wavy walled channels we observe that the spontaneous flow transition occurs at an activity smaller than the critical activity of a flat walled channel since, the undulated segments within the channel actively facilitate slip of the fluid in the bulk over their surfaces.

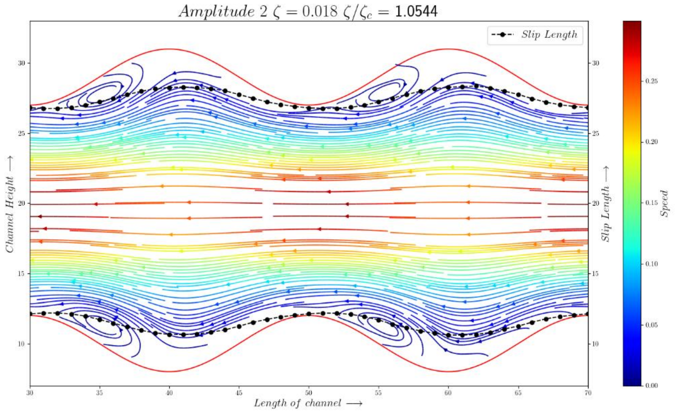

Figure 1: Streamline plot for wavy walled channel with amplitude 2, near critical activity (ζ_c).

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AM - P37

Indian Society of Rheology

Measuring entropy production in active turbulence

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Active particles like bacteria and sperm cells sustain continuous intake and dissipation of energy. Consequently, they are intrinsically out of equilibrium which leads to a non-vanishing entropy production rate (EPR) even in steady states. Quantifying how EPR varies in different collective phases is crucial for developing a thermodynamic framework for the active matter. In this work, we look at EPR in active turbulence. We use Active Model H, a continuum model used to represent active particles in a momentum-conserving fluid, to study turbulence in contractile scalar active systems. We measure the local EPR in numerical simulations, and we unveil the relation between the magnitude of entropy production and topological defects in the system. Also, we study how EPR varies with the noise intensity and activity parameters.

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Indian Society of Rheology

Ergodicity breaking in harmonically bound active dynamics

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Ergodicity breaking in anomalous stochastic processes plays an important role in revealing diffusion behavior. It comes due to the non-equilibrium properties of various complex systems like bacteria, biological cells to application-oriented self-driven particles such as Janus colloid. Here we have studied the dynamics of active Brownian particle in harmonic potential and observed a novel dynamical transition from self-similar bound trajectories to confined in annular region, resulting in non-ergodic behavior. The system undergoes a weak to strong ergodicity breaking governed by the two intrinsic timescales equilibrium time (τ_k) and the persistent time (τ_R). We have experimentally studied ergodicity in the dynamics of optically trapped Pt-coated Janus particle, and it agrees well with our numerical simulation of the Langevin equation in harmonic potential. This study is relevant to fundamental studies of various self-driven active particles and correct interpretation of the statistical data in various complex systems.

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AM - P41

Indian Society of Rheology

A Study on the Transport Properties of Active Brownian Particles in Asymmetric Ratchet Potential

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Active Brownian particles are a microscaled subclass of a wider classification called active matter which comprises particles extracting energy from the environment and converting it into mechanical work. Examples are schools of fish, flocks of birds, and herds of animals, and when coming to the microscopic scale, it includes unicellular organisms like bacteria, artificially created Janus colloids, and nanorobots. The transport properties of an active chiral Brownian particle in asymmetric ratchet potential under heavy damping are considered. The self-propelled particles lose detailed balance, and the particles generate a non-zero drift speed towards the easy flow direction, replicating a Brownian motor[1]. The average current (J_{avg}) is calculated, and the diffusivity of the particle is analyzed from the effective diffusion coefficient (D_{eff})[2]. The transport coherence is studied by the Peclet number (Pe)[3]. There is an optimum value of self-propelled velocity (v_0), at which the current is maximum. At low temperatures, the average current and effective diffusion coefficient shows multiple peaks as a function of angular velocity Ω of the chiral active particle. The graph of Peclet number reveals the occurrence of giant transport coherence, indicating highly reliable transport at moderate values of Ω

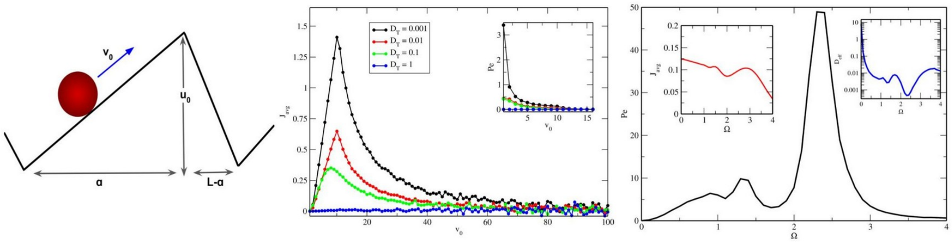

Figure 1: (a) ABP in asymmetric ratchet potential (b) J_{avg} as a function of v_0. Inset shows the Peclet number as a function of v_0. (c) Peclet number as a function of Ω. Inset shows J_{avg} and D_{eff} as a function of Ω.

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AM - P42

Colloidal transport by active dimers

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We study two simple models of active transport. In our models an active run-and-tumble particle is attached to a cargo colloidal particle. The two models we consider are: (a)Model 1 where the run-and-tumble particle is freely joined to the colloidal particle (b)Model 2 where the run-and-tumble particle attaches to the colloidal particle at a fixed angle. The dependence of the dynamics on the ratio of radii of the active and passive particle and tumble time of the run-and-tumble particle is also studied. Our study aims at finding regimes of the parameter space where transport is most efficient.

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Hydrodynamics of flagellated microswimmers in confined fluids

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Microswimmers have become an important topic of research in soft matter physics. Understanding their individual dynamics and the study of their interactions among each other and with the substrate, involve challenging physics. Confinements introduce modifications to the hydrodynamic flows and interactions, resulting in rich phenomenology and many surprising and puzzling collective behaviors. This ongoing work aims to investigate the effect of plane surfaces on the self-propulsion and interactions of flagellated microswimmers, such as bacteria, swimming near a substrate or in thin films. Using a minimal model of flagellated bacteria, we derive the flow fields around the swimmer near a substrate, considering simultaneous reflections of the flows off the cell-surface and the substrate to a good approximation. We demonstrate that the extended nature of the flagella leads to crucial hydrodynamic interactions which strongly influences the overall cell dynamics near the substrate. Detailed investigations of the cell-wall interactions and the hydrodynamic interaction between different swimmers under confinement are on-going. Our results are important to understand living and confined active matter, as well as, biological processes, such as the formation of bacterial biofilms.

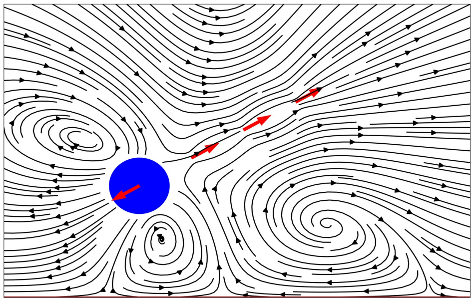

Figure 1: Streamlines of the flow field around our model microswimmer near a substrate.

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AM - P45

Indian Society of Rheology

Unveiling the propulsion dynamics of active patchy colloids using optical tweezers

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Active colloids have the ability to propel themselves in a fluid medium through self-diffusiophoresis achieved by asymmetric catalytic decomposition of H_2O_2 around the colloidal particles. The propulsion kinetics of such colloids have been extensively researched unveiling various colloidal phenomena. However, very few works have studied the self-propulsive force which controls the dynamics involved in the active propulsion. Theoretical framework for the self-propulsive force has been laid by analytically solving the Langevin equations but direct measurement of self-propulsive forces is a necessity for modelling the complex behaviour of active swimmers. In this study, we have quantified the self-propulsive forces exerted by active polystyrene microspheres at various catalytic patch coverages using optical tweezers. The catalytic patch was varied by vapour deposition of platinum catalyst at the angles of 10°, 30°, and 90° with respect to particle containing substrate. Catalytic patch coverage area was the lowest with Pt 10° colloidal batch and increased with increasing coating angles. We found that Pt 10° colloidal particles exerted the largest force of 769±79 fN against the optical trap which denoted that they had efficient propulsion even though having the least number of catalytic decomposition sites available of all other coating angles. The force data was supported with the optical tracking data where 10° coated particles traversed significantly larger displacements at same fuel concentrations. Overall, this study provides deeper insights into active colloidal dynamics that can help us develop chemical nanomotors that could efficiently replicate biomimetic motions.

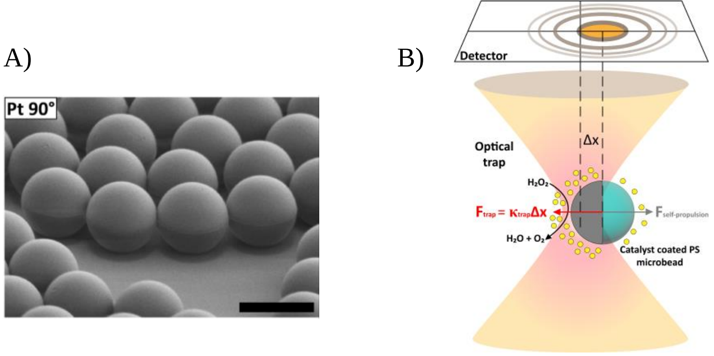

Figure 1: A) SEM image of polystyrene microspheres coated with platinum catalyst at 90°, B) Schematic of the self-propulsive force measurement using optical tweezers

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BM – O12

The effervescent cell membrane: nonequilibrium driving and active emulsions

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Abstract: Molecular organisation of the multicomponent plasma membrane of cells has long been described in terms of equilibrium physics. It is now clear that this purely equilibrium picture is inadequate and that the dynamical molecular organisation at different scales needs to be understood in terms of active nonequilibrium driving arising from the actomyosin cortex. These considerations give rise to a novel mesoscale organisation at the plasma membrane, that we term *active emulsions*, which exhibit non-reciprocity and granularity. Using active field theories and supported by experiments, I will show that the plasma membrane is a natural arena to discuss many of the key conceptual ideas in soft active matter.

BM-O1

Influence of nonequilibrium switching of segmental states on chromatin compaction

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Knowledge about the dynamic nature of chromatin organization is essential to understand the regulation of processes like DNA transcription and repair. While most models assume protein organization and chemical states along chromatin as static, experiments have shown that these are dynamic and lead to the switching of chromatin segments between different physical states. To understand the implications of this inherent nonequilibrium switching, we present a diblock copolymer model of chromatin, with switching of its segmental states between two states, mimicking active/repressed or protein unbound/bound states. We show that competition between switching timescale T_t, polymer relaxation timescale τ_p, and segmental relaxation timescale τ_s can lead to non-trivial changes in chromatin organization, leading to changes in local compaction and contact probabilities. Radius of gyration of chromatin shows a non-monotonic behavior with T_t. We find that polymers with a small segment length (N_s) exhibit a more compact structure than those with larger segment lengths. Also, we observe that the switching can lead to higher contact probability and better mixing of far-away segments.

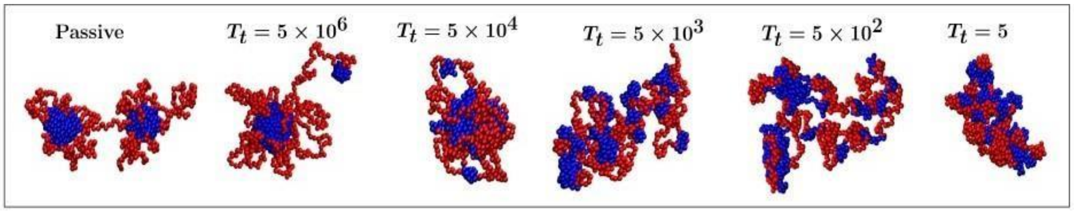

Figure 1: Steady state snapshots of the polymer for different switching time T_t and with segment length $N_s = 16$.

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BM-O8

Computing polymer properties of chromatin from contact map data

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Simulating chromatin is crucial for predicting genome organization. Using Micro-C data, we systematically coarse-grain chromatin and derive essential polymer representation quantities: bead size distributions, bond length fluctuations, and effective spring constants. Contrary to prevailing beliefs, we find chromatin beads can overlap, yielding an effective soft potential and overlap parameter. We also analyze angle distributions, revealing intrinsic folding patterns and bendability. Our study identifies two structural states and variations at Topologically Associating Domain (TAD) boundaries vs. interiors. We integrate these findings into a comprehensive polymer model, offering foundational parameters for future chromatin simulations.

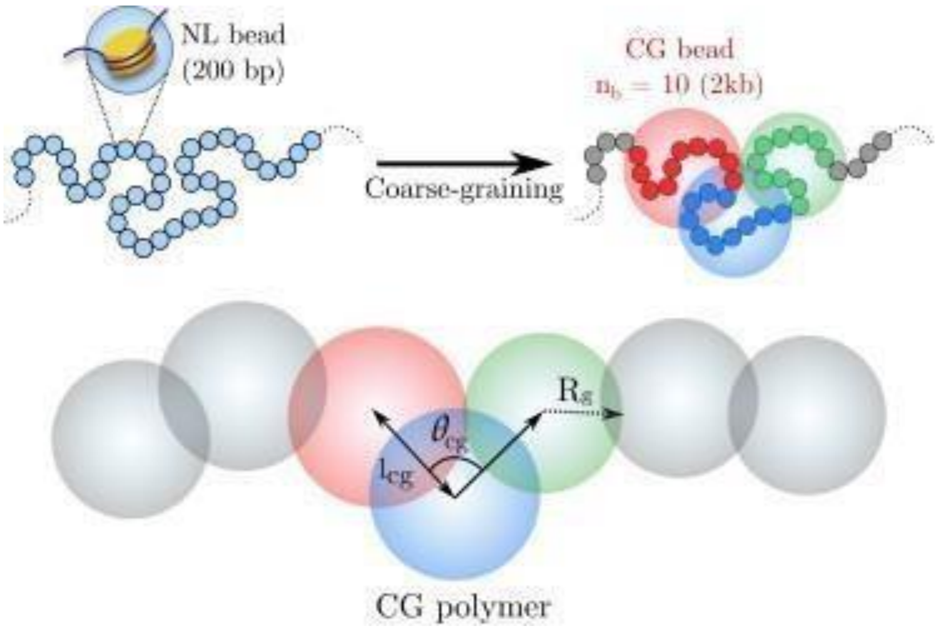

Figure 1: Systematic coarse-graining of chromatin configurations at nucleosome resolution to measure polymer properties at various genomic scales.

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Viscoelasticity of single folded protein using dynamic atomic force microscopy

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The advent of atomic force microscopy, along with optical tweezers, ushered in a new field of single molecule force spectroscopy, wherein the response of a single protein or a macromolecule to external mechanical perturbations is measured. Controlled forces ranging from pN to nN are applied to measure the unfolding force distribution of a single protein domain. In a clamp type experiment, the folded protein is subjected to a constant force to measure the unfolding time distribution. Simultaneously, there were efforts to measure the elastic and viscous response of a single domain by applying sinusoidal forces and measuring the resulting deformations produced in a bid to quantify its viscoelasticity. The deformation's phase lag with respect to the applied force provides the elastic and viscous response of the protein, akin to oscillatory rheology. Despite numerous technical advances in AFM, an artefact-free measurement of a folded protein's viscoelasticity largely remains a challenge[1]. In this talk, I will discuss efforts to measure viscoelasticity of proteins using dynamic AFM, identifying pitfalls that make these measurements elusive[2]. Finally, we discuss a new promising method, which reported viscoelasticity of a folded protein and its implications for our understanding of protein dynamics and structural flexibility [2,3].

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BM-O9

Title: Biophysical approaches to understand genome organization

Mahipal Ganji
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The DNA double helix structure is stabilized by base-pairing and base-stacking interactions. However, a comprehensive understanding of dinucleotide base-stacking energetics is lacking. In my talk, I will present about multiplexed DNA-based point accumulation in nanoscale topography (DNA-PAINT) imaging with designer DNA nanostructures that enabled us to measure the free energy of dinucleotide base stacking at the single-molecule level. We demonstrate the application of base-stacking energetics in designing DNA-PAINT probes for multiplexed super-resolution imaging, and efficient assembly of higher-order DNA nanostructures. I will also talk about our latest data from single molecule imaging of bacterial Nucleoid associated proteins (NAPs) interactions with DNA. Our data indicate that NAPs undergo co-condensation on DNA.

BM-O2

Speed variations of bacterial replisomes

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Replisomes are multi-protein complexes that replicate genomes with remarkable speed and accuracy. Despite their importance, their dynamics is poorly characterized, especially in vivo. In this paper, we present an approach to infer the replisome dynamics from the DNA abundance distribution measured in a growing bacterial population. Our method is sensitive enough to detect subtle variations of the replisome speed along the genome. As an application, we experimentally measured the DNA abundance distribution in *Escherichia coli* populations growing at different temperatures using deep sequencing. We find that the average replisome speed increases nearly fivefold between 17 °C and 37 °C. Further, we observe wave-like variations of the replisome speed along the genome. These variations correlate with previously observed variations of the mutation rate, suggesting a common dynamical origin. Our approach has the potential to elucidate replication dynamics in *E. coli* mutants and in other bacterial species.

References

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BM-O13

Single-cell morphology dictates bacterial population growth under 3D confinement

Tapomoy Bhattacharjee

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Can physical properties of the microenvironment act as selection pressures at the population-level? Our current understanding of factors that exert such effect on population growth dynamics implicates genetic mutations and chemical cues, based on experimental assays performed using homogeneous liquid or 2D cultures. However, in their natural niche, bacteria inhabit complex and disordered 3D microenvironments with diverse mechanical properties. Here, to test if the physical microenvironment can selectively favor the collective growth of certain microbial strains under 3D confinement, we design transparent porous 3D growth media that match the viscoelastic properties of natural microbial habitats. Combining optical density-based growth measurements, 3D confocal microscopy, and agent-based simulations, we find that the shape anisotropy of high-aspect-ratio bacteria provides them with a selective advantage to grow more efficiently under increased 3D confinement as opposed to spherical bacteria. More precisely, under 3D confinement, high aspect ratio bacteria produce elongated colonies with larger surface areas allowing them to access nutrients more effectively. Our work provides an example of how the alteration in the physical of the microenvironment can dictate the microbiome composition in 3D disordered materials. This will help in understanding and modeling population dynamics within microbial

communities inhabiting diverse biological niches using elementary physical principles.

Lipid Vesicles Adhesion Mediated by the Sugar-Cleaving Enzyme Invertase

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We discuss the invertase-induced generation of membrane tension arising from its binding to the outer leaflet of the GUV bilayer membrane. Figure 1 illustrates a cross-section of the GUV surface having an attached invertase that has been labeled with fluorescent dye (green). The relevant shape deformations [1] and membrane fluctuations [2] of GUV with and without bound invertase are quantified. Contact angle measurements of the adhered GUVs to the substrate reveal a change in membrane tension that depends on the concentration of the bound protein in the passive and active state.

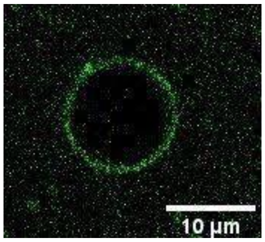

Figure 1: Adhered GUV planar cross-section tagged with Invertase (green).

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Antibiotic-Induced Bacterial Membrane Dynamic Alterations unraveled by Super-Resolution Nanoscopy

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Antibiotics play a crucial role in combating bacterial infections, but their excessive and improper use has led to the emergence of antimicrobial resistance (AMR). Bacteria exposed to sub-lethal concentrations of antibiotics have been observed to develop the resistance for the drug they are exposed to. Since various drugs target the bacterial membrane directly or indirectly, understanding the response of the bacterial membrane becomes crucial. Our research, employing Fluorescence Correlation Spectroscopy (FCS), has revealed that *E. coli*'s membrane (model membrane) becomes more fluidic with a higher diffusion coefficient after the addition of antibiotics[1,2]. Moreover, growing *E.coli* in progressively increasing concentrations of antibiotics enables it to survive even at the minimal inhibitory concentration (MIC) and the concentration higher than the MIC. Interestingly, the onset of colistin resistance appears to occur relatively quickly at a specific concentration. To delve deeper into these mechanisms, we utilized super-resolution stimulated emission depletion (STED) nanoscopy coupled with FCS[3]. Our findings demonstrate the emergence of length scale dependent dynamical changes in the membrane as antibiotic concentrations increase, starting from sub-MIC levels. This indicates that *E. coli* attempts to adapt its membrane to sustain growth even at the MIC value. Our AFM results show different patterns of roughness of the outer membrane during the process of the bacteria being allowed to grow at different antibiotic concentrations. These interesting results can be an important step in understanding how this gram-negative bacterium tries to develop antimicrobial resistance at short time scales upon exposure to antibiotic.

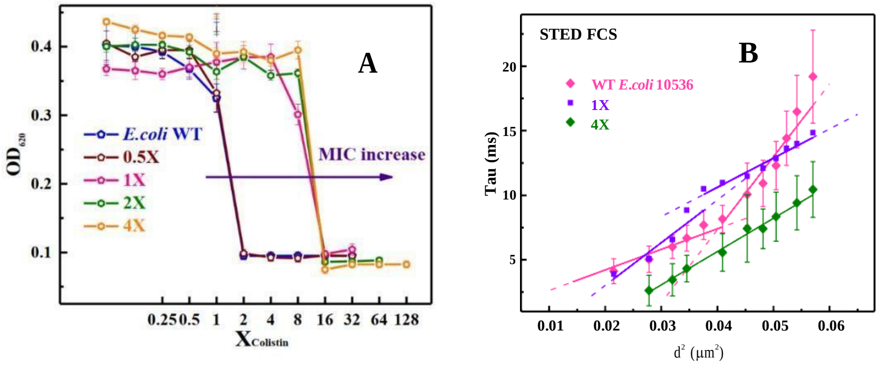

Figure 1: (A) MIC graph for the pristine *E.coli* 10536 and in response to varying concentrations of a specific antibiotic (B) STED-FCS graph for pristine *E.coli* and bacteria incubated at different concnentrations of antibiotic.

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Elucidating the Multifaceted Nature of Multiphasic Condensates in Neuronal Diseases

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Active droplet formation or biomolecular condensation has emerged as an effective means for cells to preserve their spatiotemporal coherence while carrying out a plethora of essential biological functions. These exquisitely regulatable supramolecular condensates are thought to form via a multitude of transient, multivalent, intermolecular forces that sequester intrinsically disordered proteins and other biomolecules into liquid-like membrane-less compartments. Aberrant liquid-to-solid transitions inside these phase-separated condensates, however, give rise to numerous neurological disorders. In our study, we present that tau and prion (PrP), two familial neuronal proteins, undergo complex coacervation fueled by domain-specific electrostatic interactions to form highly dynamic, mesoscopic droplets. To investigate the behavior comprehensively, we employ a unique combination of time-resolved tools in conjuncture with single-molecule spectroscopy, covering an extensive range of timescales, from nanoseconds to seconds. We uncover a symphony of molecular events associated with the formation of heterotypic condensates comprising ephemeral, domain-specific, short-range electrostatic nanoclusters. We also show that upon aging, tau:PrP condensates gradually convert into solid-like hetero-assemblies via persistent intermolecular interactions which is the hallmark of neuropathological diseases. Additionally, our results show RNA can transform these heterotypic condensates into multiphasic assemblies ranging from core-shell structures to nested droplets reminiscent of hierarchically organized multi-layered cellular bodies. In conclusion, our study underscores the ubiquitous occurrence of condensate immiscibility in diverse biological systems. This intriguing revelation serves as a model to engineer self-organized synthetic compartments, and precisely modulate complex biomolecular processes. Moreover, I will also discuss my recent work which focuses on interactions and the effect of protein quality control machinery on tau phase separation and pathology further enriching our understanding of these intricate cellular processes.

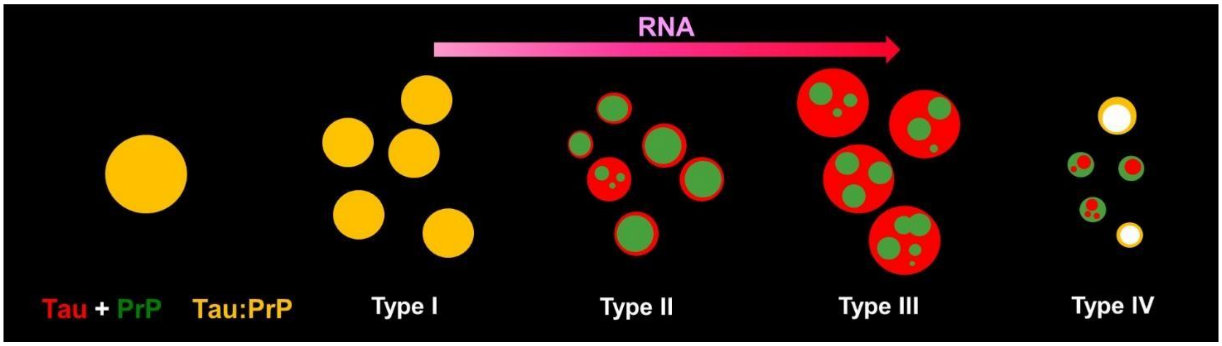

Figure 1: Schematic illustration of morphological transformations during complex phase separation of tau, PrP, and RNA.

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BM-O5

Indian Society of Rheology

Pattern formation by living droplets in chemoattractant gradients

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Gradients of extracellular signals organise cell behaviour in tissues. Although we have good models for chemotaxis of isolated cells in signal gradients, it is not clear how cells react to gradients when the cell population is undergoing 3D morphogenesis, in which cell-cell interactions and cell-signal interactions undergo extensive emergent behaviour. Using light sheet imaging to simultaneously monitor signalling, single-cell and population dynamics in Dictyostelium cell populations, we show that these cells migrate towards nutritional gradients in swarms. As the swarm advances, it deposits clumps of cells at the rear, triggering their differentiation. Clump deposition is explained by a model in which the cell swarms behave as living droplets, with cell proliferation and signal gradient remodelling opposing surface tension to promote droplet shedding. The model predicts vortex motion of the cells within the droplet emerging from active forces, which was validated by 3D tracking of single cells in the swarms. Our data and modelling show how the emergent dynamics of multicellular communities cause qualitative differences in chemotaxis from isolated or non-interacting cells.

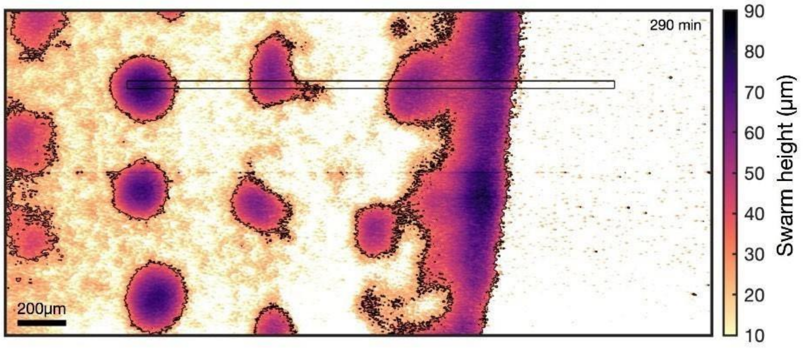

Figure 1: Pattern formation by Dictyostelium cells via chemotaxis and feeding (viewed from above).

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BM-O6

Emergent spatiotemporal multistability enabled by the bio-mechanical underpinnings of different gene regulatory network motifs

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Spatiotemporal pattern formation plays a key role in various biological phenomena including Epithelial Mesenchymal Transition (during cellular differentiation and cancer initiation). Though the reaction-diffusion systems enabling pattern formation have been studied phenomenologically, the bio-mechanical underpinnings of these processes has not been modeled in detail. Here, we present the emergence of multistable spatiotemporal patterns due to transcriptional/cooperative gene regulation, host-circuit interaction, and protein dimerization. We investigate the patterns formed due to the coupling of inherent multistable behavior of transcriptional toggle switch es(bistability), toggle triads (tristability), coupled with their molecular diffusion, with varying diffusion coefficients, across a two-dimensional tissue. In another setup of diffusible cellular environment, we investigate emergent spatiotemporal bistability by a motif with non-cooperative positive feedback, that imposes a metabolic burden on its host. Spatiotemporal diffusion coupled with competitive protein dimerization and autoregulatory feedback induces higher order spatiotemporal multistabilty — quadra-, hexa-, and septastabilty. These analyses offers valuable insights into the design principles of synthetic bio-circuits, and suggest mechanistic underpinnings of biological pattern formation.

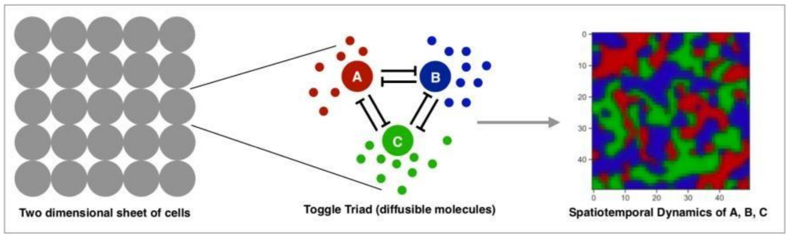

Figure 1: Illustration for **spatiotemporal tristability** – toggle triads with diffusing molecules embedded in a monolayer of cells, mimicking a biological tissue

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The hierarchical structure and complex rheology of mucins

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Mucins represent an important class of glycoprotein with a distinct structural motif – a peptide linked backbone surrounded by a bottlebrush of charged sugar residues. These biomacromolecules function as soft wet barriers in vertebrate physiology in a range of solvent conditions: salt, pH and water content [1]. By virtue of domains involving hydrophilic/hydrophobic, hydrogen bond and electrostatic interactions, they have a propensity to form cross-links leading to higher level aggregates, and networks [2].

In this work, we study the dilute dispersions of a commercial pig gastric mucin (PGM). Shear and oscillatory rheology exhibit Herschel-Bulkley type shear thinning and gel-like type III behaviour respectively, reminiscent of colloidal sols. Herein, the mucin aggregates are visualized as colloidal particles with a complex internal morphology of bottlebrushes. Interestingly, the system undergoes continuous aggregation followed by sedimentation when left unperturbed at room temperature for longer times (~ 24 hours), especially predominant in solvents with varying ionic strengths. Insights on the time evolution and local heterogeneity of the microstructure are obtained from small angle X-ray scattering (SAXS) studies. Extended small angle neutron scattering (USANS, SANS [3-5]) of the well mixed samples in deuterated solvents were sensitive to the radius of gyration of mucin particles, electrostatic interactions between the particles, and more importantly the electrostatically mediated intra-particle mucin chain correlations. Dynamic light scattering revealed the effect of size distribution, and overall surface charge of mucin particles on the colloidal-scale aggregation. Hence, we probe the hierarchy of structure over length-scales many orders in magnitude to comprehend the structure-property relationships in mucins.

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Indian Society of Rheology

Decoding of temperature signals by the thermosensory neurons in *Caenorhabditis elegans*

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The nervous system plays a crucial role in the survival of biological organisms, especially in changing environmental conditions. In general, specific types of neurons sense and transduce external stimuli through various signaling pathways [1]. Mathematical models along with the experimental studies of these processes help us understand how signals are decoded and transmitted in living organisms.

In this poster, I shall discuss a mathematical model that aids in understanding how a pair of thermosensory neurons in small nematodes *C. elegans* detect changes in external temperature. Experimental studies on neuronal thermosensation have demonstrated the gene-specific activation of a cGMP signaling pathway in response to thermal stimuli. Our model focuses on three key elements of this pathway: receptors, inhibitors and voltage channels, and provides an understanding of the effects of a variety of external perturbations on the temporal dynamics of second messenger cGMP and calcium. We show that partial or complete inactivation of the key entities of the pathway alters the response levels of calcium. Additionally, the process of interaction between different entities of the signaling pathways is influenced by cellular noise and is stochastic in nature [2-3]. Accounting for the influence of this heterogeneity-induced stochasticity in our model helps us provide some key insights into the temperature-mediated calcium responses in the thermosensory neuron of *C. elegans*.

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Homeostasis in confined environments

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Morphogenic processes during embryonic development involves a complex interplay of coordinated cell behaviours on length scales significantly larger compared to that of an individual cell. During these morphogenic events, it is essential that the epithelium maintains a fine balance between the divisions and ingressions of cells [1]. Moreover, the intercalations induced due to the cell division and ingression assists in tissue fluidisation, consequently, morphogenesis [2]. For instance, inhibition of cell divisions is found to inhibit the formation of primitive streak in the chick embryo [2, 3]. At present, the mechanical principles underlying the establishment of homeostasis in confinement remains poorly understood. In this study, we employ vertex model simulations [4] to understand the establishment of homeostasis in confined environments. We consider a random tiling and actively grow the cells with a constant growth rate by scaling the preferred area of the cell. Cells are divided or ingressed based on the cell area using probabilistic approach. Moreover, by coupling the division and ingression process to local stress field we examined the correlation between the homeostasis and stress in the monolayer. Our analysis unveils the factors that influence cell divisions and ingressions, consequently homeostasis in confined environments.

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BM-P2

Yeast Budding Dynamics in Complex 3D Environments

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The colony growth of budding yeast (*Saccharomyces cerevisiae*) has been extensively studied in 2D systems, observations from which have been linked to biochemical cues and genetic pathways. However, both, the natural habitat as well as the widespread commercial applications of yeast involve complex viscoelastic 3D environments, which present a dramatically different mechanical regime than typically realized using conventional liquid or flat plate cultures. Our present study seeks to bridge this gap by investigating yeast growth dynamics in 3D viscoelastic media, wherein we seek to understand how the stiffness of the culture matrix affects yeast growth. To investigate this, we use 3D growth media with precisely tuneable material properties. Combining absorbance-based growth assays with live-cell confocal imaging, we find that the budding times of yeast dramatically vary between environments of different yield stresses. We intend to investigate cellular-level dynamics that induce this change in behaviour and seek to study the effect of microenvironments on yeast growth dynamics.

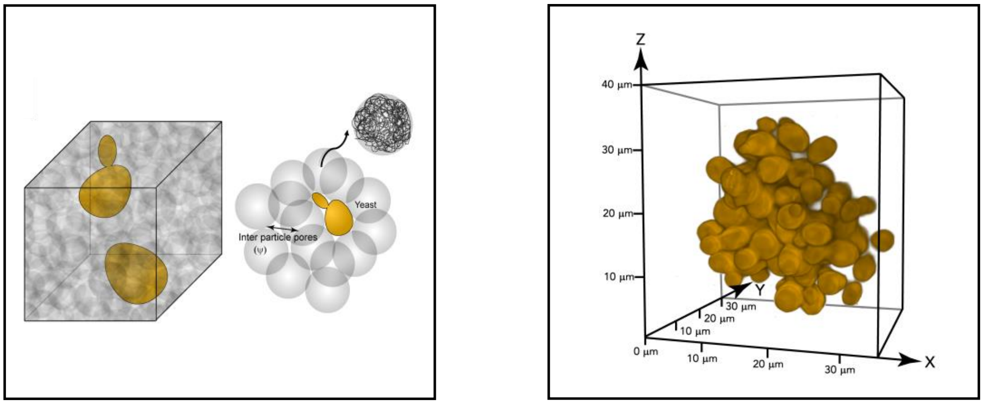

Figure 1: Yeast growth inside viscoelastic environments

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BM-P3

Cellular growth and behavior in designer 3D culture media

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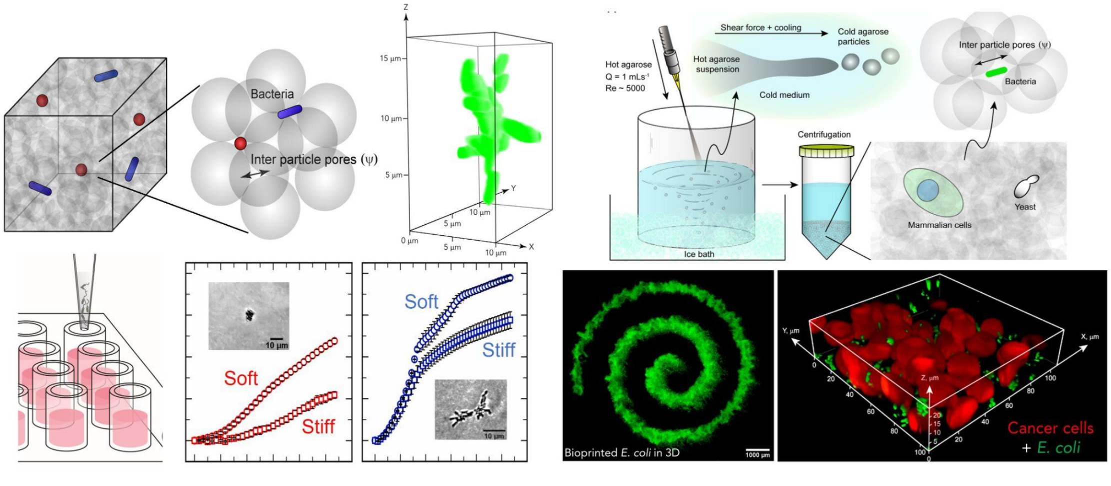
How do altered substrate properties affect the growth of different bacterial species in 3D? Bacterial growth has been extensively studied in homogeneous liquid or flat plate cultures. However, in nature, bacteria inhabit complex niches such as soil, tissues, and mucus, which are granular and porous three-dimensional microenvironments. To test if the physical properties of such disordered 3D microenvironments affect bacterial growth dynamics, we design transparent porous 3D growth media that match the viscoelastic properties of natural microbial habitats. Combining growth measurements with 3D confocal microscopy and agent-based simulations, we find that the shape anisotropy of rod-shaped bacteria provides them with a selective advantage to grow more efficiently under increased 3D confinement as opposed to spherical bacteria. Our study presents a generic model of how single-cell morphology is a key determinant of collective organization in 3D space. Parallelly, our work reveals critical limitations of commercially-sourced polyelectrolyte microgels, which sequester antibiotics and biologically important ions. Additionally, they require complex synthesis protocols which severely limit their broader accessibility. We overcome these challenges using a high-throughput strategy to synthesize charge-neutral agarose-based microgels, which serve as a versatile growth media for 3D cell culture and 3D bioprinting [1]. We leverage this platform for bacterial, yeast, and long-term mammalian cell culture and live imaging, antibiotic selection, cell encapsulation, 3D bioprinting of live cells, and spatiotemporal sampling. Our one-step synthesis approach presents a promising and highly accessible platform for studying cellular interactions and dynamics in porous 3D environments, as well as for organoid culture and tissue engineering applications.



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Location and Concentration of Aromatic-Rich Segments Dictates the Percolating Inter-Molecular Network and Viscoelastic Properties of Ageing Condensates

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Maturation of functional liquid-like biomolecular condensates into solid-like aggregates has been linked to the onset of several neurodegenerative disorders [1]. Low-complexity aromatic-rich kinked segments (LARKS) contained in numerous RNA-binding proteins can promote the aggregation process by forming inter-protein β-sheet fibrils that accumulate over time—ultimately driving the liquid-to-solid transition of the condensates [2]. However, key open questions such as how the behavior of individual molecules within condensates, and their intermolecular interactions, change over time; or if we can rationally design protein sequence modifications to prevent ageing, remain open [3]. In this study (Fig. 1), we combine atomistic Molecular Dynamics simulations with sequence-dependent coarse-grained models of various resolutions [4,5] to investigate the role of LARKS abundance and position within the amino acid sequence in the maturation of biomolecular condensates. We find that the location of the LARKS motifs along the protein sequence crucially determines the rate of cross-β-sheet transitions and the associated loss of liquid-like behavior over time. Our simulations show that shifting the location of the LARKS-containing domain in *fused in sarcoma* (FUS) protein towards its center slows down condensate aggregation. More strikingly, our simulations further predict that adding RNA to FUS with re-located LARKS fully inhibits the accumulation of β-sheet fibrils, maintaining functional liquid-like behavior without ageing [6]. Taken together, this work sheds light on a key area of research aiming to advance our molecular understanding of condensate ageing, which is needed to design novel therapies to prevent age-related diseases caused by condensate dysregulation.

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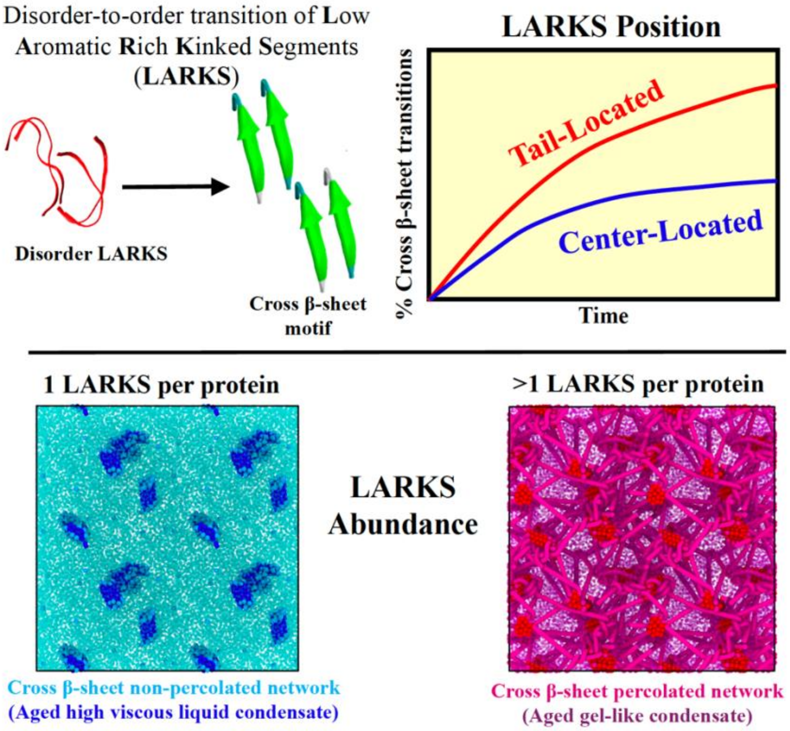

Figure 1. Graphical abstract of the research presented above.

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BM-P5

Disruption of Alzheimer’s Amyloid-β Fibrils: Insight from all-atom Molecular Dynamics Simulation Study

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Alzheimer’s Disease (AD) is a progressive, neurodegenerative, geriatric and multi-faceted in nature with genetic, environmental and some unknown mechanism associated with it. Amyloid-β (Aβ) fibrils have been reported to be the principal clinical hallmark due to its direct involvement in the neurotoxicity and degeneration leading to AD. The therapeutic approaches have been broadly classified into (i) inhibition of the aggregation of the Aβ monomers and (ii) disaggregation of the preformed Aβ fibrils. The use of β-sheet breakers, nanoparticles, small molecules and natural compounds have been studied for the same purpose. The failure of the clearance of the drugs from inhibition strategy has motivated the in-depth investigations for the disaggregation approach. In this view the role of natural compounds has been preferred owing to their natural intoxicity and biocompatibility with the human system.

Various natural compounds from different category have been selected for the destabilization studies: caffeine from alkaloids; caffeic acid, gallic acid, epigallocatechin and ellagic acid from polyphenols; omega-3 polyunsaturated fatty acids (PUFAs) and lycopene from terpene. We have applied Molecular Dynamics (MD) simulation to study the destabilization potential along with the mechanistic details. In all the natural compounds, a general observation towards destabilization is drifting of the terminal chain from the fibril. Among all the polyphenols, ellagic acid (REF) has been found to be the best binder and destabilizer of Aβ fibril wherein it binds to chain A of the fibril by accessing fibrillar cavity. The amphiphilic nature of the PUFAs was found to be the supportive for the better binding with the fibril, wherein polar head binds to the positively charged residues and long carbon tail to the hydrophobic residues of the fibril. The lycopene was found to interact with the surface and cavity of the fibril depending on the architecture of the fibril. From all the studies, the major governing principles behind destabilization of the fibril was observed by loss of H-bonds, breakage of salt-bridges, loss of hydrophobic interactions and loss of β-sheet content. A similar trend also has been observed with other small molecules as well as polypeptides. We have also observed that the destabilized structure does not refibril upon elimination of the ligand from the system. Thus, the present study successfully establishes the efficacy and prophecy in the destabilization of preformed Aβ fibril as a promising therapeutic approach for treating AD.

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BM-P6

ROLE OF TISSUE MECHANICS IN WOUND HEALING IN AN EPITHELIAL MONOLAYER

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Wound healing is a natural biological process by which the body of an organism repairs and restores damaged or injured tissue. It involves a sequence of various cellular and molecular processes. Wound healing is essential for maintaining the structural integrity of the body as well as for protection from infections and the external environment. In the past, wound healing has been studied on model organisms like mouse, zebrafish, frog, as well as on flies like Drosophila melanogaster. Besides these, in vitro studies on wound healing have been performed using MDCK monolayers (kidney epithelia), HaCaT cells (keratinocytes), CaCo-2 (colon epithelial cell line), and so. During these studies, people have looked at the biochemical components or molecular mechanisms involved in wound healing or the role of cell-substrate interaction or cell-substrate interaction combined with tissue mechanics in wound closure. However, the contribution of various geometrical constraints and tissue mechanical properties alone to wound healing is unclear. Upon making experimental wounds using MDCK monolayer, we found that irrespective of the wound fraction, the total number of cells surrounding a wound determines its fate. Motivated by this, we have developed a mathematical model based on vertex model equations to study the mechanical response of a wounded epithelial monolayer to specific geometrical and mechanical parameters. Using this model, we predict three stationary phases of wound closure by tissue mechanics alone– a closing phase, a shrinking phase, and an expanding phase.

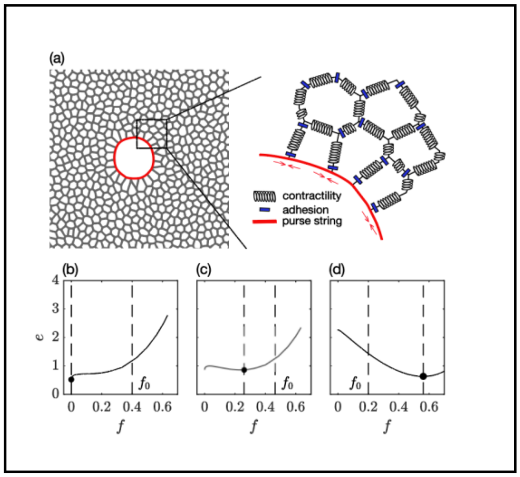

Figure 1: (a) Schematic showing wounded epithelial mono-layer. Energy per cell (e) as a function of wound fraction (f), with a given initial wound fraction (f_0) (b) for a closing wound. (c) for a shrinking wound. d) for an expanding wound.

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BM-P7

Topology-driven spatial organization of ring polymers under confinement

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Entropic repulsion between DNA ring polymers under confinement is a key mechanism governing the spatial segregation of bacterial DNA before cell division. Here we establish that “internal” loops within a modified-ring polymer architecture enhance entropic repulsion between two overlapping polymers confined in a cylinder. Interestingly, they also induce entropy-driven spatial organization of polymer segments as seen *in vivo*. Here we design polymers of many different architectures by introducing a minimal number of cross-links between specific monomers along the ring-polymer contour. If the polymer in consideration is the DNA of *E.coli*, then the cross-links are likely introduced by various bridging proteins inside the living cell. We use Monte-Carlo simulations to investigate the segregation of two polymers with modified topologies confined in a cylinder, which initially had spatially overlapping configurations. This helps us to (a) identify the architectures that lead to higher success rates of segregation and (b) establish the mechanism that leads to localization of specific polymer segments. We use the blob model to provide a theoretical understanding of why certain architectures lead to enhanced entropic repulsive forces between the polymers as well as the polymer segments. This polymer physics mechanism [1] has been used to explain the emergent spatio-temporal organization of bacterial chromosomes of *E.coli* as they undergo replication and segregation. This entropy based mechanism can reproduce spatio-temporal organization as seen in slow growing bacterial [2] cells as well as in more complex fast growing bacterial cells [3] with overlapping cell cycles.

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Entropic insights on emerging traits from growing bacterial colonies

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Since the first agglomerations of single cell microorganisms which made life possible on the planet Earth, microbes have demonstrated prolific ability to adapt to changing environments, thanks to their emergent traits. Yet, beyond the species-specific traits, to date we lack a general mechanistic understanding of the adaptive traits, and the underlying biophysical principles driving their spatiotemporal adaptivity. We build up on our recent discovery that phenotypic noise self-regulates growth and collective structural organization [1] to understand the principles of emergence utilizing a thermodynamic framework. Using a novel custom-built label-free algorithm, we track single cells transforming into colonies of surface-associated bacterial species and reveal the formation of distinct sub-colonies comprising descendants of individual bacterial cells. The analyses of the emerging intra-colony dynamics demonstrate that progeny chains of cells form *enclaves* within the colony, displaying a spatial affinity for close relatives, at the cost of reduced intermixing – an entropically favorable option. These enclaves - deeply intertwined with the dynamics of topological defects in the colonies - display a high degree of self-similarity with the colonies at large on several key phenotypic traits. A remarkable feature of this enclave scale intermixing that we uncover is the dependence of the spatial geometry of intermixing on the level of biological activity in the colony. These far-from-random arrangements of cells in such colonies - a distinct yet unifying feature of pattern formation in nature - uncovers several so-far hidden features of emergent organization within bacterial colonies at intermediate scales, ultimately pointing at the biological benefits of proximity to close kith and kin, despite higher entropic costs [2].

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Homo- versus Hetero-Oligomerization Drives the Thermo-Osmo Responsive Behavior of the Enterobacterial Sensory Protein H-NS

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Environmentally regulated gene expression is critical for bacterial survival under a variety of conditions including extremes in temperature, pH, osmolarity, and nutrient availability. Sensing the environment is orchestrated by macromolecules with diverse underlying mechanisms - e.g. changes in protein oligomerization status, unfolding, or DNA superhelicity - that eventually regulate gene expression in a finely tuned manner. Here, we dissect the thermo- and osmo-responsory behavior by H-NS, an archetypal sensory protein ubiquitous in enterobacteria. Employing an array of experimental spectroscopic, calorimetric, hydrodynamic methods and computational modeling, we show that H-NS exhibits a large degree of heterogeneity in its helical content and oligomeric nature with osmolarity- and concentration-dependent populations of monomer, dimer, tetramer, and octamer. The population of distinct oligomeric species is controlled by an intricate interplay between dimerization and oligomerization, which are dictated by two different sites on the protomer. This, in turn, drives competition between weak homo- versus hetero-oligomerization of protein-protein and protein-DNA complexes, which is also tuned in a concentration-dependent manner by the co-repressor Cnu. Additionally, H-NS forms liquid-like condensates at low concentrations of DNA, and even in the absence of DNA but at high concentrations. Rationally engineered mutations and a phosphor-mimetic variant dramatically suppress oligomerization and phase separation. Our work thus uncovers important organizational principles that act at different length scales in H-NS to ultimately determine its response to environmental cues in a finely tuned manner.

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BM-P11

Understanding Phase Separation Characteristics of Non-Amyloid β-Component of α-Synuclein

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Biomolecular condensates are membrane-less assemblies consisting of proteins and nucleic acids. Altered protein dynamics can however lead to pathogenic condensates linked to several neurodegenerative diseases. Numerous studies have reported Liquid-Liquid Phase Separation (LLPS) to be the key mechanism resulting in the formation of biomolecular condensates. During LLPS, a homogeneous mixture spontaneously separates into a dilute and a dense phase and coexist. Multivalent interactions of Intrinsically Disordered Proteins (IDPs) are major drivers of phase separation. α-Synuclein is an IDP consisting of 140-residues whose aggregated states are associated with Parkinson’s disease. It consists of a non-amyloid β-component (NAC) region (residues 61-95) which is prone to beta sheet formation. Available data suggest that NAC plays a crucial role in the formation of pathogenic condensates. In this work, we have employed all-atom molecular dynamic simulations to investigate the phase behaviour of NAC region in water. Temperature replica exchange molecular dynamics simulations have also been performed to explore the phase change characteristics of NAC. This study will aid in further understanding the role of different domains of α-Synuclein in phase separation.

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Conformation and Charge - Density Dependent Phase Separation and Ageing of an Intrinsically Disordered Protein

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Intrinsically disordered domains are known to facilitate multivalent interactions driving protein phase separation and potentially aggregation. Here, we employ a model system, the intrinsically disordered DNA binding domain (DBD) of Cytidine Repressor CytR, to design macromolecular assemblies and/or condensates whose physical properties can be tuned by various factors (temperature[1], osmolarity[2], mutations[3], and crowding[4]). Our preliminary work on CytR and its mutants reveals a conformation - dependent differential phase separation behavior, aggregation and droplet solubilization. Specifically, we find that the excess positively charged CytR, which samples an excited helical folded state and exhibits weak helicity in its native ensemble, displays time dependent conversion from droplets to aggregates in the presence of anionic polyphosphate. The mutant P33A, a fully unfolded variant with no helical content, exclusively undergoes only aggregation with polyphosphate. On the other hand, the A29V/A48M mutant which is fully folded, primarily forms droplets which then solubilizes within three hours. We thus showcase how charge-density, in addition to net charge, drives differential phase separation of a disordered protein.

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Indian Society of Rheology

Molecular dynamics investigation of the dynamical response of the interfacial waters near DPPC bilayer to Hyaluronic acid

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Hyaluronic acid (HA) is a long, hydrophilic polyanion that aids in cellular contact, coating of cellular surfaces, and lubrication. It is overexpressed in cells and body fluids during pathogenic situations like colon cancer. Previous studies have shown that the interaction between HA and lipid molecules is mediated by water molecules. The dynamic properties of the interfacial waters are critical to understand spectroscopic data and the mechanical properties of the HA-lipid complexes. However, there is no report on the theoretical understanding of HA's significance in water dynamics near lipid vesicles. To that end, we take Dipalmitoylphosphatidylcholine (DPPC) lipid bilayer and HA of different sizes and concentrations in our fully atomistic molecular dynamics simulation. Our findings suggest that at the HA-DPPC bilayer interface, HA restricts the translational and rotational diffusion of the water molecules. We note the signature of heterogeneity in the dynamics of water. We explain our results based on the inherent hydrophilic nature and the network structure of HA molecules at the interface.

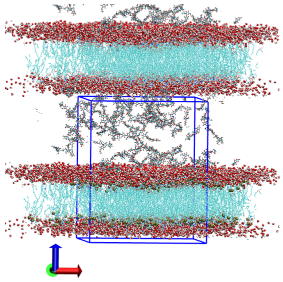

Figure 1: Model of the simulated system. Interfacial water molecules (red VDW representation) are shown along with HA(Licorice) and lipid bilayer (cyan Bonds).

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BM-P14

Protein Association Reaction Study on GB1 Protein Dimerization in a Crowded Environment

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Protein associated states are crucial in regulating functions such as DNA binding, immune response, enzymatic reactions, signal transduction. Recent studies indicate that the macromolecular crowders, that occupy 30-40% of the intracellular environment, can significantly favor the formation of protein self-aggregated complexes, whereas some crowders even impart a destabilizing effect on protein-protein complexes. In this work, we investigate dimerization of Immunoglobulin-binding protein G of the B1 domain of the Streptococcus species in presence of lysozyme crowders using Martini coarse-grained model. Simulations are biased with metadynamics and parallel tempering methods to ensure convergence of the free energy of binding. Our analysis shows that dimer formation is destabilized in presence of lysozyme crowders and the domain-swapped dimer of GB1 protein is more likely to be formed in both with and without crowder systems. The findings are compared with that obtained from a low-resolution CG model from ReaDDy simulations, the scaled particle theory model and the available experimental results.

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Role of WASP in Arp2/3 complex activation

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Actin filament branching is a fundamental cellular mechanism generating forces necessary for lamellipodia and filopodia formation critical for cell migration and motility. Filament branching is nucleated on the sides of preexisting actin filaments by Actin-Related Protein 2/3 (Arp2/3). Arp2/3 protein, natively found in inactive state, is activated by nucleation promoting factors (NPFs). Arp2/3 adopts a barbed end like conformation and binds to the actin mother filament to function as a nucleation seed for daughter filament growth [1,2]. The role of NPFs and actin filaments in the activation of Arp2/3 and the conformational rearrangements occurring during Arp2/3 activation remains highly debated. In this work, we present a molecular dynamics study investigating Arp2/3-NPF interactions at molecular scales. By sampling inactive-active state transition using well-tempered metadynamics simulations we find that the energy barrier impeding short-pitch conformational transition of Arp2-Arp3 results from the interaction of subdomain 2 of Arp2 with the “bumper helix” in Arp3. Further, using a coarse grained heteroelastic network model derived to reflect the correlated fluctuations observed at atomic resolutions [3], we aim to capture the slow “soft” modes of the multidomain protein resulting in the activation of Arp2/3 complex. Overall, using atomistic and coarse grained simulations, our study provides molecular insights to unravel the mechanism of Arp2/3 activation.

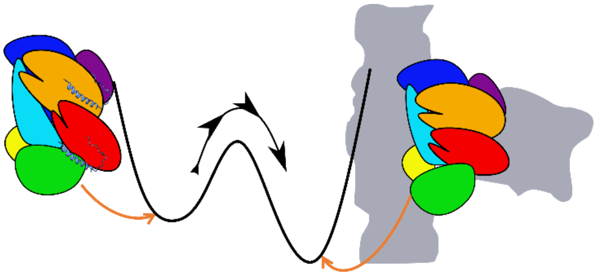

Figure 1: Schematic of mechanism of Arp2/3 activation.

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BM-P17

pH mediated aggregation and fibrillization of amyloid beta(16-22)

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Protein aggregation in the brain is a hallmark of neurodegenerative diseases.Amyloid beta is a protein with 38-42 residues that has been linked to Alzheimer's disease. Aggregates of this protein, which primarily consist of cross beta sheet structures, can form as a result of changes in a variety of environmental factors such as salt concentration, pH, temperature, and so on.According to research, the brains of Alzheimer's disease patients have an acidic environment due to mitochondrial dysfunction and lactic acid accumulation, which may have played a role in promoting protein aggregation[1–3] . This protein's residues 16-22, also known as the KLVFFA cluster, are responsible for the formation of cross beta sheet structures[4]. In this study we investigated the aggregation kinetics of this short peptide of amyloid beta protein containing residues 16-22 over a pH range of 4.5-9.The short peptide's aggregation kinetics were compared to the kinetics of proteins containing 38, 40, and 42 residues, respectively. The fibrils that form are imaged using TEM, SEM, and AFM. Secondary structure content analysis was also performed on all protein sequences using FTIR spectroscopy.We also investigated this protein cluster's propensity to form liquid liquid phase separated (LLPS) droplets in the presence of polyphosphate, a biopolymer essential to the functioning of living organisms. Understanding the fibrillization pathway of these proteins can help us develop new therapeutic strategies.

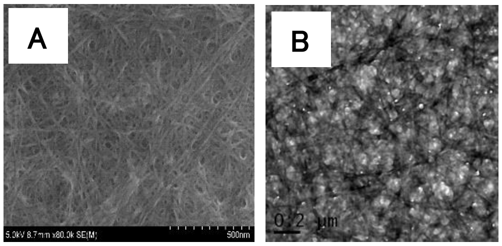

Figure 1: (A) SEM and (B) TEM micrographs showing fibrils formed by amyloid beta(1-40)

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Association of Globular and Intrinsically Disordered Proteins in Particle Based Coarse-grained Models

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Particle-based coarse-grained models are routinely used to to understand the influence of cellular environment on protein-protein association. Here we employ an interacting particle based reaction-diffusion simulation strategy to obtain the free energy of association of globular and intrinsically disordered proteins (IDPs) under crowded conditions. The globular protein system consists of two B1 domain of protein G (GB1) monomers undergoing association in presence of protein crowder lysozyme. The interaction between GB1 and lysozyme is modelled with a Lennard-Jones potential having varying potential depth to understand the effect of attractive potential strength on the free energy change. In the IDP system, activation domain of the steroid receptor co-activator 3 (ACTR) and nuclear co-activator binding domain of CBP/p300 (NCBD) are considered in presence of polymer crowder polyethylene glycol (PEG), where the IDPs and PEG interact with a harmonic repulsive potential. The change of free energy due to crowding for globular proteins show opposite sign in comparison with experiments [1,2], whereas for IDPs, the results show similar sign although the magnitude is reduced. Based on these results we propose how particle-based models can be improved to study crowding effects on globular proteins and IDPs.

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BM-P19

Single-droplet single-molecule FRET and vibrational Raman scattering reveal conformational heterogeneity and shapeshifting within liquid condensates

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Phase separation of biomolecules into liquid-like supramolecular assemblies has newly emerged as a critical organizing principle within living cells. The intrinsically disordered group of proteins (IDPs/IDRs) comprising low-complexity (LC) have been identified as the major drivers of cellular phase separation leading to the formation of these non-canonical MLOs involved in diverse physiological functions and fatal neurodegenerative diseases. Hence, obtaining insights into critical molecular events rendering the formation of these pathological assemblies has gained significant importance. Here, we illuminate the inner workings and chain dynamics of an archetypical prion-like, low-complexity domain of Fused in Sarcoma (FUS-LC) using an amalgamation of single-droplet, single-molecule FRET, picosecond time-resolved fluorescence anisotropy, fluorescence correlation spectroscopy in conjunction with vibrational Raman spectroscopy. We investigate the change in material properties accompanying a density transition coupled percolation of the monomeric FUS-LC, leading to the formation of a dense phase comprising a viscoelastic network fluid. I will discuss the outcomes of our studies, highlighting the presence of co-existing subpopulations and their interconversion, along with the translational and rotational dynamics within the dispersed and droplet phases of the FUS-LC domain.

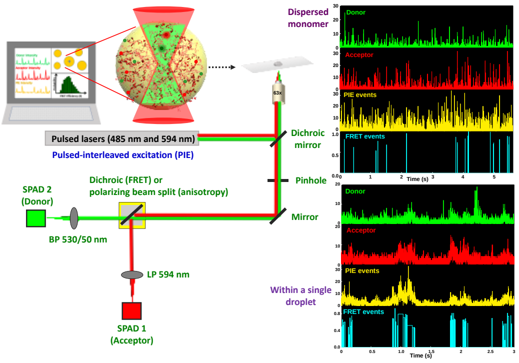

Figure 1: Experimental design for single-droplet single-molecule measurements.

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Complex coacervation of a prion-like protein and a J-domain protein into multiphasic condensates inhibits the amyloid formation

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Eukaryotic cells organize a wide array of biochemical processes by creating membrane-bound organelles in a spatiotemporal fashion to function properly. In addition to this, cells also contain membrane-less organelles (MLOs) or biomolecular condensates formed via liquid-liquid phase separation (LLPS) that are primarily composed of intrinsically disordered proteins/regions (IDPs/IDRs) and nucleic acids. These biomolecular condensates are involved in a myriad of critical cellular processes and are implicated in various devastating neurodegenerative diseases. [1,2] However, the phase separation of proteins inside the cell is tightly regulated to maintain the metastable state of these condensates and prevent any excessive abnormal aggregation. These MLOs consist of a wide range of J-domain proteins (JDPs) which can play an important role in modulating the sequence of events that govern the intracellular phase transition into liquid-like droplets, further preventing pathological amyloid aggregation. This regulation process by JDPs remains largely unexplored. Utilizing a multidisciplinary approach involving a diverse range of biophysical, molecular biology, and imaging tools, I have initiated my studies aimed at characterizing the role of conformational dynamics, heterogeneity, and intermolecular contacts that governs the heterotypic condensation of a prion-like protein and a JDP into liquid droplets. Furthermore, I will discuss our recent results on the LLPS of these proteins into liquid-like droplets, which can effectively impede the formation of fibrous pathological aggregates.

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BM-P21

Investigating the Chaperone Mechanism of α-Crystallin in Preventing γD-Crystallin Aggregation in Cataract Formation

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Cataract, a leading cause of global blindness [1], arises due to the aggregation of crystallin proteins within the eye lens, leading to opacification and loss of transparency. Although present at a high concentration of up to 450 mg/ml, crystallin proteins remain soluble, maintaining lens transparency and the refractive index [2]. Chaperone proteins, particularly α-crystallin, play a vital role in preventing the aggregation of these proteins [3]. However, the specific molecular interactions between α-crystallin and other crystallin subtypes, such as γD-crystallin, which is one of the most abundant crystallins in the human eye lens, remain poorly understood.

In this study, we aimed to elucidate the interactions between the α-crystallin's ACD [4] domain and the domains of γD-crystallin. To achieve this, we employed a multifaceted approach combining molecular docking, interaction studies, molecular dynamics simulations, and Markov state modeling-based free energy calculations. Through molecular docking studies, we first probed the binding affinity and specificity of the ACD domain with the domains of γD-crystallin. Subsequently, we conducted detailed interaction studies to gain insights into the key residues and molecular forces driving the stable complex formation. To quantify the thermodynamic stability of the α-crystallin-γD-complex, we calculated the free energy of binding, comparing it to the stability of γD-crystallin in the absence of ACD. Our findings shed light on the energy landscape and the role of the ACD domain in mitigating the aggregation process of γD-crystallin, a crucial step in cataract formation. Furthermore, we harnessed molecular dynamics simulations to explore the dynamic behavior of the ACD-γD complex over extended time scales. These simulations allowed us to investigate the conformational changes and fluctuations occurring within the complex and provided valuable insights into its overall stability.

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Exploring the molecular aspects of α-crystallin's inhibitory role against γD-crystallin aggregation

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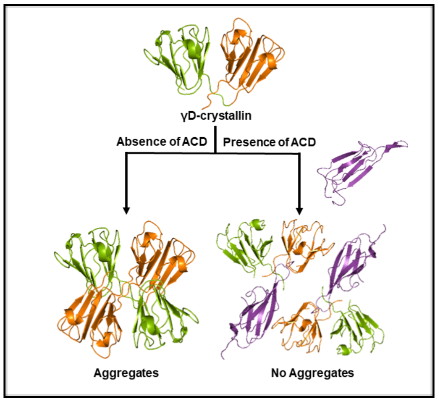
Cataracts, a major cause of global blindness, contribute significantly to the overall prevalence of blindness. Opacification of the lens, which results in cataract formation, primarily occurs because of the aggregation of crystallin proteins within the eye lens. Despite the high concentration of these crystallins, they remarkably maintain lens transparency and refractive index. α-crystallins (α-crys), acting as chaperones [1], play a crucial role in preventing crystallin aggregation, although the exact molecular mechanism remains uncertain. In this study, we employed a combination of molecular docking, all-atom molecular dynamics simulations, and advanced free energy calculations to investigate the interaction between γD-crystallin (γD-crys) [2], a major structural protein of the eye lens, and α-crys protein. Our findings demonstrate that α-crys exhibits an enhanced affinity for the NTD2 and CTD4 regions of γD-crys. The NTD2 and CTD4 regions form the interface [3] between the N-terminal domain (NTD) and C-terminal domain (CTD) of the γD-crys protein. By binding to the interface region between the NTD and CTD domains of the protein, α-crys effectively inhibits the formation of domain-swapped aggregates and mitigates protein aggregation. Analysis of the Markov State Models using molecular dynamics trajectories confirmed that the minimum free energy conformations correspond to the binding of the ACD to NTD2 and CTD4 that form the inter-domain interface.



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Predictive Modeling of Biological Enzyme-Substrate Binding: Understanding Conformational Dynamics and External Influences

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Understanding the intricate process of enzyme-substrate binding is of paramount significance in both biological and industrial contexts [1][2]. In recent times, significant progress has been made in identifying binding pockets, also known as active sites, within enzymes [3]. However, the comprehension of the conformational changes that enzymes undergo during substrate binding remains a critical challenge. These changes vary substantially between different enzymes, and even within a specific enzyme, the binding pockets may exhibit variability depending on the nature of the substrate. Furthermore, external factors such as temperature [4], pH [5], and the presence of other molecules can exert profound effects on this mechanism [6]. In light of these challenges, this study aims to construct a cutting-edge machine-learning model using a comprehensive dataset gathered from molecular dynamics simulations and molecular docking studies. By leveraging these advanced computational techniques, we endeavor to gain deeper insights into the dynamic nature of enzyme-substrate interactions and unravel the intricacies of their binding mechanisms.

The primary objective of our research is to develop a robust machine-learning framework (Figure 1) capable of predicting enzyme-substrate interactions with exceptional accuracy and generality. By incorporating data obtained from molecular dynamics simulations and molecular docking experiments, we expect our model to capture the dynamic behavior of biological enzymes during the binding process. This holistic approach will allow us to comprehend the underlying patterns that govern the binding pocket dynamics and recognize how different external factors influence the enzyme's behavior. The significance of this study extends to multiple domains such as drug designing, enzyme engineering, bioremediation, food biotechnological processes, and biomedical research, leading to more sustainable and efficient industrial practices.

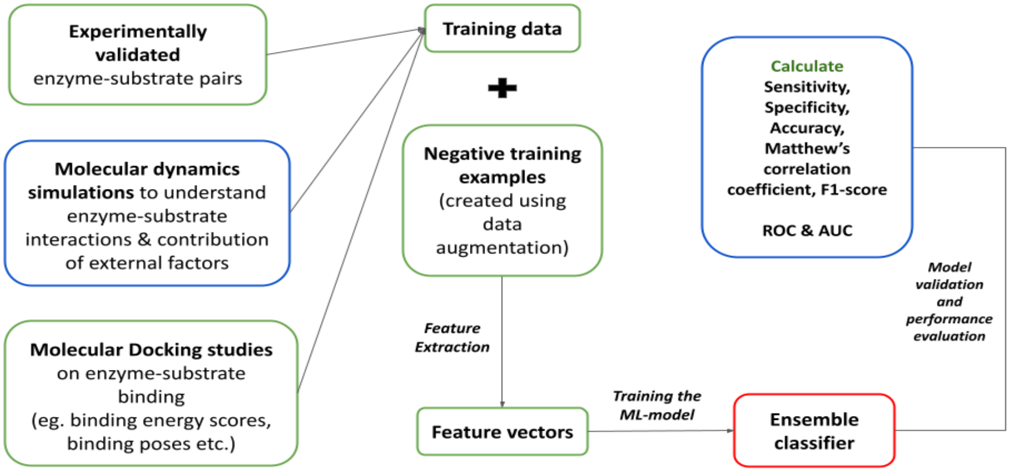

Figure 1: The model architecture.

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Liquid-liquid phase separation of p53 and its paralogs p63 & p73 in the context of cancer progression.

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p53 is a tumor suppressor protein and regulates the transcription of a broad range of downstream genes. The p53 gets sequestered in cells with succeeding stages of cancer as amyloid[1]. The p53 amyloids possess almost all the characteristics of a prion and have the potential to transform normal cells into tumorigenic cells by altering the cell cycle and proliferative pathways [2,3]. Under normal conditions, the activation and functional consequences of the protein are correlated with its phase separation inside the nucleus and in the cytoplasm. Interestingly, two other family members of p53, i.e., p63 and p73, have near-identical functional properties and form phase-separated entities inside the cell. Like p53, these two proteins also sequester inside the cancer tissues[1]. The functional consequences of these two proteins under phase-separated conditions are unexplored. Moreover, how the p63 and p73 get sequestered in cells is yet to be understood in a tumorigenic context. In addition to this, how p63 and p73 cellular condensate modulate the p53 condensate functions are yet to be uncovered in the context of cancer progression. We over-express p63 and p73 proteins in the p53-null cell line by introducing the genes transiently and characterizing the condensate behavior inside the cell either in the presence or absence of p53. Additionally, we explore the functional consequences of the proteins in condensate, either normal or disease condition.

In accordance with the in-cellular condensate characterization, we study the condensate behavior of the proteins in vitro with a simple two or three component-system. This allows us to understand the effect of several biomolecules on the modulation of condensate properties of these proteins.

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Indian Society of Rheology

Multicomponent membranes with active recycling: compositional inhomogeneities and morphology

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Organelle membranes are multicomponent fluid sheets that undergo recycling through fission and fusion process. The impact of this recycling process on the morphology and local composition is still not very well understood. Here, we use a method recently developed by us[1], using dynamically triangulated surface model, to mimic the membrane activity. We report results from the simulations of a three-component vesicle composed of 1) active species which can have non-zero spontaneous curvature and participate in recycling and 2) inactive species which do not participate in recycling. These active species are of two types and induces curvature of opposite sign when attached to membrane. We investigate the steady state morphologies as a function of activity rate, spontaneous curvature and the strength of interaction between species. We find an intriguing strong dependence of morphology on the preferred curvature of the species undergoing recycling.

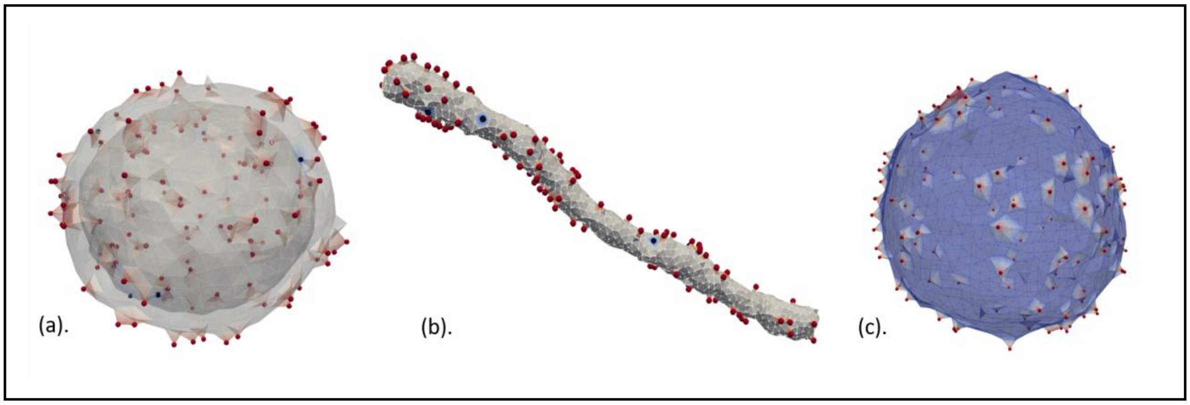

Figure 1: Snapshot of morphologies at the steady state observed for the ratio of active species with positive and negative spontaneous curvature, 97:3. Morphology given in Fig. 1(a), 1(b) and 1(c) are for same rate of addition of particles with positive curvature but the addition rate of negative species was varied (0.00001, 0.0001 and 0.02) so as to look at the impact of different addition rate. The shapes shown are Stomatocyte, Tubular and Vesicle respectively.

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Indian Society of Rheology

Amylin modulates the electrical properties of Amyloid-β during its fibril growth

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Abstract

The proton transfer via hydrogen bonds facilitates protein activity and accelerates many reactions requiring charge transfer or electronic signaling mechanisms. Herein, we study the amylin (hIAPP) mediated modulations in the electrical properties of Amyloid-β (Aβ) aggregation under a temperature gradient of 5 ^{0}C (40-35 ^{0}C) using impedance spectroscopy. We recently showed that proton transfer's activation energy can monitor the changes in fibril growth directions in real time by relating sub-nm-scale proton hopping (NPH) through Aβ and hIAPP aggregates to their structural features. These proteins having aromatic residues are qualitatively shown here to execute both NPH and multi-scale proton hopping (MPH) during their aggregation. We use 200 ns molecular dynamics simulations, molecular docking, and photoluminescence emission spectra to show that Aβ and hIAPP aggregation are MPH and NPH-dominated systems, respectively. Further, the scenarios where NPH/MPH dominates over MPH/NPH were investigated by monitoring the electrical conductivity of Aβ and hIAPP solutions in different molar ratios. Their aggregation gives rise to different proton conduction pathways (wire), and intra- and inter-aggregate proton hopping may lead to both positive and negative activation energy of proton transfer with respect to the buffer. The positive and negative activation energies for proton transfer were related to the protein aggregates, facilitating and hindering proton conductance structural features. These structural features predicted by electrical measurements of these peptides were corroborated with FTIR measurements. The electrical properties of Aβ-hIAPP aggregation may help understand their implications in Alzheimer's disease.

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Impedance spectroscopy revealed the surfactant-driven unfolding and refolding of a globular protein.

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The interaction between proteins and surfactants results in the formation of protein-surfactant complexes that find numerous applications in the food, cosmetic, and pharmaceutical industries. Proteins interact differently with ionic and non-ionic surfactants. The interaction is influenced by electrostatic and hydrophobic forces. Ionic surfactants unfold globular proteins, while non-ionic surfactants are better for refolding denatured proteins. In this work we employed impedance spectroscopy (IS), a label-free method, to investigate the unfolding and refolding of human serum albumin (HSA), a globular plasma protein, in the presence of sodium dodecyl sulfate (SDS), an anionic and polysorbate-20 (Tween-20), a non-ionic surfactant. Using a 20 mV rms AC voltage, the impedance spectra were recorded throughout a frequency range of 50 Hz to 1 MHz. We examined the dielectric properties of HSA in 10 mM phosphate buffer saline, with an emphasis on altering the concentration of co-dissolved surfactants. To obtain the equivalent electrical analog circuit, the electrical response of the IS data is fitted using EIS spectrum analyzer. To analyze the conformational changes of surfactant-driven HSA, the behavior of charge transfer resistance (R_{CT}) is used as a convenient parameter. The results obtained through IS align well with those obtained from Dynamic light scattering, near- and far- UV Circular dichroism, and Photoluminescence spectroscopy.

Keywords: Circular Dichroism, Dynamic light scattering, Human serum albumin, Impedance Spectroscopy, Photoluminescence Spectroscopy.

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BM-P30

Signatures of glassy dynamics in liquid-ordered lipid membrane

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Lipid domains in bilayers have often been explored as an essential component in multiple physiological functions like assemblage of proteins, signalling and pathogen entry, to name a few. Computational studies on membranes are often challenging since the emergent behaviours occur across a wide range of time- and length-scales. The studies on lateral lipid dynamics thus far, have observed that the heterogeneity is attributed to lipid diffusion which resembles glassy dynamics [1]. Here we have utilised a non-affine parameter χ 2 which measures the extent of deformation in local lipid geometry. It has been previously shown to perform well in distinguishing ordered and disordered phases in model membranes [2]. It also established solid spatial and temporal correlations with physical measurements such as particle displacements, non-gaussianity and overlap functions [3], in a model glass system like the binary Kob-Anderson system. Since membranes exhibit a similar phenomenon, we try to capture heterogeneity in diffusion dynamics of lipids in a model membrane system that is predominantly in liquid ordered phase.

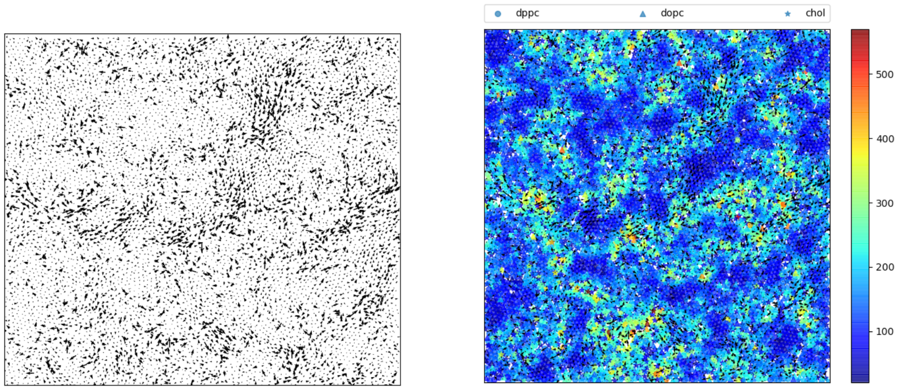

Figure 1: (a) Particle displacement profile and (b) overlap of NAP values in Lo membrane model (DPPC/DOPC/CHOL) at T288 K

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BM-P31

Smearing Technique For Liquid Viscosity Measurement

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Film coating, especially the blood smear coating are common techniques for generating thin films, or blood smears for monolayer analysis of the film. In such processes, a reservoir of the coating fluid is entrained between a substrate and a blade, where the blade is held at an angle above the substrate and is moved at a certain speed. The movement of the blade drags the entrained liquid thereby generating a thin film. We have built a simple device to cast a thin liquid film on to a glass slide with the aid of a moving blade held at an angle over the substrate (Fig. 1). The present work compares the film generation on a smear device with a model based on a Landau−Levich theory. The device operates at different constant speeds and based on the speed; one can generate desired films with a thickness gradient. We also show that the device has the capability of generating uniform thickness films by varying the operating speed. The model can also predict the viscosity of the film cast on the substrate by the measurement of the film length. Hence, the smearing device is effectively able to generate desired thickness films in addition to predicting viscosity. The device can hence find its application as a bed-side diagnostic tool in medical diagnostics and disease detection where a simple blood smear can be used in the estimation of the whole blood viscosity.

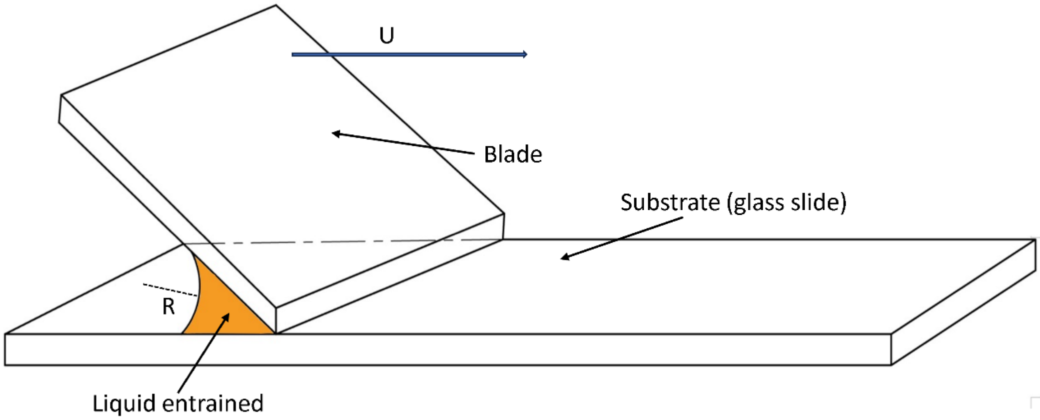

Figure 1: Smearing device schematic.

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Dynamics of Bacterial Biofilm Growth on Porous Surfaces: Insights from a Three-Phase Model

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We employ a three-phase model to investigate the growth dynamics of bacterial biofilms on solid substrates. The three phases are the cell, extracellular matrix (ECM), and nutrient-rich aqueous phases. We use the thin-film approximation as the characteristic biofilm height is much smaller than the biofilm's radius to simplify the model. We numerically solve for the biofilm height, volume fractions of each phase, and nutrient profiles in the biofilm. We consider the effect of osmotic flow on dynamic behavior. Our model establishes that the ECM phase primarily generates internal osmotic pressure, promotes nutrient flow, and facilitates biofilm growth and swelling. Additionally, our results suggest that increased cell and ECM growth leads to faster expansion due to increased biomass, while increased surface tension forces redistribute biomass radially.

We compare our model predictions of expansion radius and velocities with experimental data from previous studies [1-2]. This confirms the critical role of osmotic-driven expansion in the growth and spreading of bacterial biofilms on solid substrates.

This study contributes to the development of strategies that will prevent biofilm formation on medical devices and other surfaces.

Keywords: Biofilm formation, Thin-film approximation, Marangoni effect, Front instability.

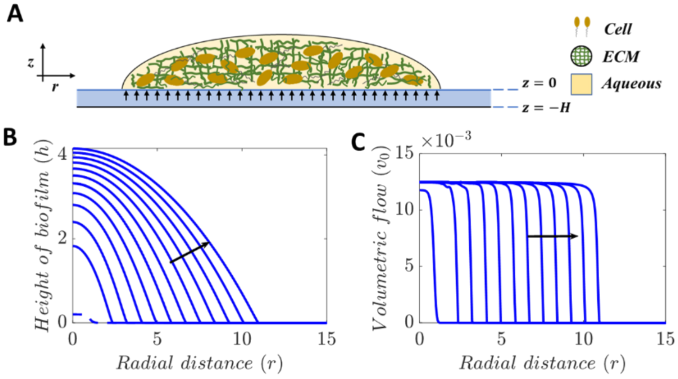

Figure 1: (A) Schematic of a bacterial biofilm on agar surface. The schematic of different phases is represented on the right-hand side. B) Numerically obtained height of biofilm (*h*). C) Variation of the osmotic influx (*v0*) within the biofilm. The solution profiles are plotted in an increment of *t=8*.

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Nanoscale Dynamic Interplay of SARS CoV Fusion Peptides and Lipids in Host Cell Entry

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The severe acute respiratory syndrome coronavirus (SARS-CoV) causes the recent pandemic of COVID-19. It enter host cells by fusing the viral & host plasma membrane using the fusion peptide of the Spike glycoprotein [1]. Several studies have been done to understand the interaction mechanism using different techniques like fluorescence spectroscopies [2], neutron reflectometry (NR) etc. However, the influence of lipids and cholesterol on peptide confirmations, penetration depth and more fundamentally the reason for SARS CoV 2 being a major infectious disease threat compared to SARS CoV 1 is still lacking. A real cell plasma membrane poses a lot of challenges with its heterogeneous complex environment, therefore, using model membranes (Composition: DPPC: DOPC: DOPS: Cholesterol (POSC) 40:34:6:20) with co-existing Liquid ordered (Lo) and disordered (Ld) lipid domains & variety of techniques from super-resolution STED microscopy with fluorescence correlation spectroscopy (STED-FCS) and Lifetime Imaging (FLIM) provides a versatile platform to probe nanoscale lipid dynamics and lipid-peptide interactions with high spatial and temporal resolution. In our study, we have employed a range of fluorescent lipids probes to investigate the distinct and specific contributions of these lipids during the fusion process. Diffusivity (D) and the Lifetime (τ) values from Lo & Ld phases are getting to similar values with increasing peptide concentration (Fig 1 (B)). Our findings suggest fusion peptides can decrease the mobility gradient not only between Lo & Ld phases, but also at different nanoscale dynamical length-scale and redistribute cholesterol from the Lo phase to the Ld Phase in order to promote the fusion process. We are also using the tagged peptides to find the possible confirmation & penetration depth into the host cell membrane. Moreover, our research aims to compare between SARS CoV 1 & 2 fusion peptide by mapping the mobility & lifetime to understand how it regulates membrane fusion events.

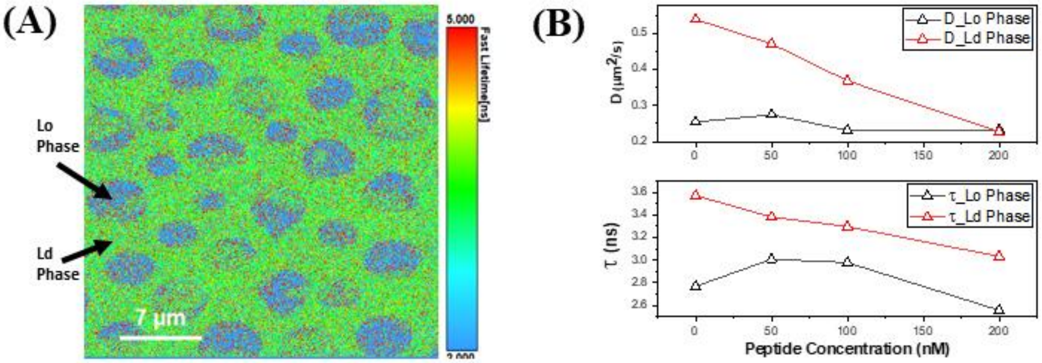

Figure 1: FLIM images of (A) Pristine POSC tagged with Atto 647N-DMPE and (B) Diffusivity measured by Confocal FCS methods (top) & Lifetime (bottom) values of with peptide concentration.

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Pulling Short DNA with Mismatch Base Pairs

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Due to misincorporation during gene replication, the accuracy of the gene expression is often compromised. This results in a mismatch or defective pair in the DNA molecule (James et al. 2016). Here, we present our study of the stability of DNA with defects in the thermal and force ensembles. We consider DNA with a different number of defects from two to sixteen and study how the denaturation pro-cess differs in both ensembles. Using a statistical model, we calculate the melting point of the DNA chain in both the ensemble. Our findings display different manifestations of DNA denaturation in thermal and force ensembles. While the DNA with defects denatures at a lower temperature than the intact DNA, the point from which the DNA is pulled is important in force ensemble.

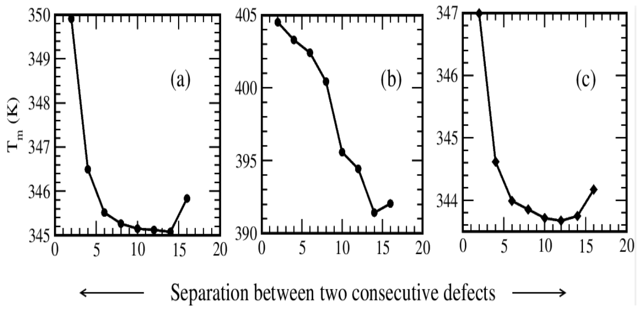

Figure 1: (a) The change in the melting temperature with the change in separation between the two consecutive defects, (a) for the homogene-ous DNA chain, (b) for the DNA chain with first half with AT pairs and second half with GC pairs, (c) for the DNA chain with alternating AT and GC pairs.

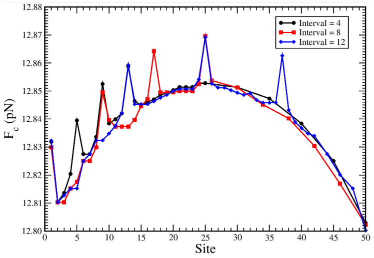

Figure 2: Critical force for a homogeneous DNA chain of 50 base pairs.

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BM-P35

Synthesis of highly biocompatible surface-modified MoS_2 Nanoflowers: unraveling the detailed antibacterial mechanisms

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The development of multi-drug-resistant bacterial infections seriously threatens public health, so efforts are needed to develop a new class of safe and effective antibacterial agents. Two-dimensional molybdenum disulfide (MoS_2) based nanostructures have great potential as antibacterial agents, but their aggregation limits their further biomedical applications. Here, we report a bio-inspired synthesis of surface-modified MoS_2 nanoflowers (NFs) with a nature motif that show good colloidal stability in aqueous media. The formation of surface-modified MoS_2 NFs has been confirmed using XRD, SEM, TEM, XPS, FTIR, and TGA analysis. The antibacterial activity of as-prepared MoS_2 NFs examined over gram-negative *Escherichia coli* and gram-positive *Staphylococcus aureus* bacteria shows inhibition of nearly 97% and 90%, respectively. The antibacterial mechanistic insights suggest the production of reactive oxygen species (ROS)-dependent and ROS-independent oxidative stress. The ROS-dependent and ROS-independent oxidative stresses were measured using flow cytometry and fluorescence imaging using DCFH-DA staining, and Ellman's assay, respectively. Our study suggests that the combined effect of both ROS-dependent and ROS-independent oxidative stress leads to enhanced antibacterial activity. Moreover, the toxicity studies towards mammalian cell lines suggested the high biocompatibility of these as-synthesized NFs, with cell viability of nearly 90%. Our study indicates that the proper surface modification can enhance the colloidal stability and antibacterial potency of MoS_2-based nanomaterials for further applications such as antibacterial coatings, water disinfection, and wound healing.

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Understanding the role of convective mixing on aerosols deposition in lung acini

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The lung is a complex organ in the respiratory system, composed of a dichotomously bifurcating tree-like network that spans over 23 generations or bifurcations. The tree terminates in tiny air sacs, known as alveoli, which protrude from the bronchioles' surface after the airway's generation. They progressively become numerous towards the generation. These alveoli expand and contract during respiration, enabling the necessary gas exchange with the bloodstream. The seminal experiment [1] on 17 healthy male subjects uncovers the existence of convective mixing in the lung acinus. In this study, we model the flows in the alveoli through experiments and simulations using the T-section to understand the role of asymmetry in the expansion-contraction of alveoli on convective mixing. We find the finite fold and stretch in the pattern formed by passive particles (dye in the experiment) with the finite asymmetry ϕ, which do not reverse after an oscillation cycle, increasing the pattern's total length. The increase in line length becomes exponential for high ϕ and lower Strouhal values (Sr) due to the multiplication of folds, which is not the case otherwise (as evident in Figure 1). We indicate exponential and linear growth regions in the parametric space of ϕ and Sr. Here, Sr is the scaled frequency of oscillation. The exponential growth leads to the chaotic mixing of particles with the residual air in the lung. Above findings would help learn the residence time of pathogens in the lung and engineer efficient pharmaceutical aerosols.

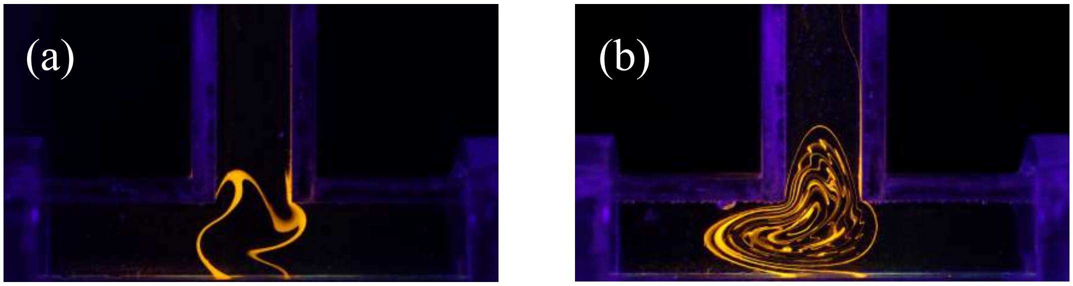

Figure 1: Deformed dye pattern after 10 oscillations: (a) for $\phi = 5°$ and $Sr = 1$ (b) for $\phi = 90°$ and $Sr = 0.5$.

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Understanding Mucin-Albumin assembly using microrheology

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Mucus is a viscoelastic layer, which is found along the lining of various organs such as the eyes, nose, mouth and the entire GI tract. The function of the mucus layer differs with its location in the body. For example, in the intestines, it protects the epithelial cell layers from the pathogens and creates a microenvironment which balances the normal gut microflora thereby facilitating a symbiotic relationship. Alteration of the rheology of the mucus layer leads to various disease conditions such as cystic fibrosis, Crohn’s disease, and gastric ulcers, among others. Mucus consists of various mucins along with proteins such as immunoglobulin, lysozyme, and albumin. In the present study[1], we explore the effect of pH on the interactions between bovine serum albumin (BSA) and porcine gastric mucins using diffusing wave spectroscopy (DWS). The study shows that BSA actively binds with mucin to form mucin–BSA complexes, which is largely driven by electrostatic interactions.

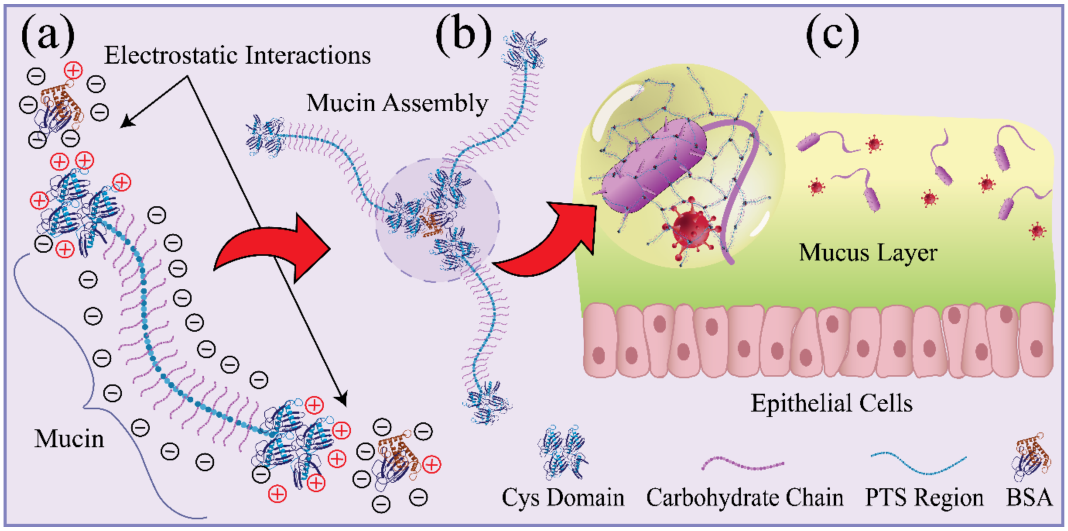

Figure 1: Caption of the Figure.

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PNIPAAm as A Thermosensitive Drug Delivery System for Targeted Cancer Treatment: A Molecular Dynamics Study

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Polymeric drug delivery systems have shown promise as platforms for targeted anticancer treatments because they provide better drug bioavailability, fewer adverse effects, and more therapeutic efficacy. For controlled drug release, poly(N-isopropyl acrylamide) (PNIPAAm) distinguishes apart from such polymers because of its thermo-responsive characteristics. Using molecular dynamics (MD) simulations at two different temperatures, 300K and 310K, we explore the potential of PNIPAAm as a drug carrier for the anticancer drug doxorubicin and also to increase the doxorubicin's drug efficacy on the targeted tumor site. We investigated the doxorubicin-polymer interactions in the aqueous environment, focusing on the influence of temperature on the release rate. The drug release kinetics and diffusion behavior analyses within the polymer matrix offer insightful knowledge of the controlled drug release mechanism.

Furthermore, we examine the conformational changes and solvent interactions of the PNIPAAM polymer at both temperatures, revealing light on its structural integrity and response to environmental changes. We intend to clarify the effect of temperature on the lower critical solution temperature (LCST) of PNIPAAm, which is essential in drug release control, by examining the system at 300K and 310K. The outcomes of this investigation demonstrate the potential of PNIPAAM as an effective drug carrier for doxorubicin in treating cancer. The atomic-level details of the drug-polymer interactions, drug release kinetics, and thermoresponsive behavior of PNIPAAm are revealed by molecular dynamics simulations. The results demonstrate the potential of PNIPAAm as a temperature-sensitive drug delivery system and emphasize the significance of temperature in influencing the drug release rate.

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BM-P39

Indian Society of Rheology

Probing the formation of pre-fibrillar prion peptide oligomer with atomistic molecular dynamics simulation

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Abstract. The structural basis of pre-fibrillar prion peptide aggregation and identification of possible intermediates still eludes us [1]. Knowledge regarding the early stages of fibril formation in atomistic detail may provide suitable information for rational drug design. In this work, using human prion peptide ^{127}GYMLGS^{132} as a model [2], we studied the oligomer formation process from dimer (O_2) to hexamer (O_6) by employing molecular dynamics with explicit solvent. The results obtained from our study indicate that the oligomer formation initiates from antiparallel β-sheet-like dimers. The successive addition of unstructured monomer was found to affect the free energy landscape of aggregation. Analysis of the free energy profile showed that the conformational transition of the aggregates initiates during tetramer (O_4) formation. The higher-order aggregates (O_5 & O_6) were found to reorder into steric-zipper, β-barrel-like structures and reside in two energy states separated by a small energy barrier. Unlikely, the lower order aggregates (O_2 & O_3) were found to remain in single deep minima with extended β-sheet structure. Hydrophilic interaction is found to be a key contributor to stabilizing the higher-order aggregates and supports the further growth of oligomers. However, the initial association of the monomers is mainly governed by transient interchain hydrogen bonds. The insights obtained from the study will help in understanding the physicochemical forces and role of interfacial water molecules for the initial formation of toxic prion oligomers.

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Indian Society of Rheology

Super-hydrophobic surface assisted micro-droplet drying for aerosol evaporation analysis

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Droplet aerosol transmission has been touted as the major contributor to airborne transmission during the recent Covid pandemic. Focus has shifted to sub-100 micron droplets as the carriers of viruses, which stay airborne for longer and can traverse greater distance. Furthermore, as the droplets originate from physiological fluid, if they dry completely before reaching ground, they turn to droplet nuclei, which will have even longer air persistence. So it is important to know the droplet nuclei physical parameters to obtain deeper understanding of airborne transmission.

Studies have been performed where the final droplet diameter size has been estimated for different droplet size, originating from physiological fluids such as saliva[1,2] or a surrogate suspension[3]. These studies employed levitation setups to obtain airborne spherical droplets and the ratio of final to initial droplet diameter (shrinkage ratio) after drying was reported to be 0.2 to 0.25.

In our approach, we have employed a super-hydrophobic (SH) surface (contact angle >150°) to obtain spherical droplets which is relatively simpler to establish. We also produced sub-100 micron sized droplets, which are the most potent carriers in airborne transmission [4]. Our obtained shrinkage ratio for these micron scale droplets were comparable in value that of previous studies[1,2,3], and we performed these experiments for saliva and different surrogate suspensions (i.e. same mass fraction solutions of NaCl, glucose and BSA).

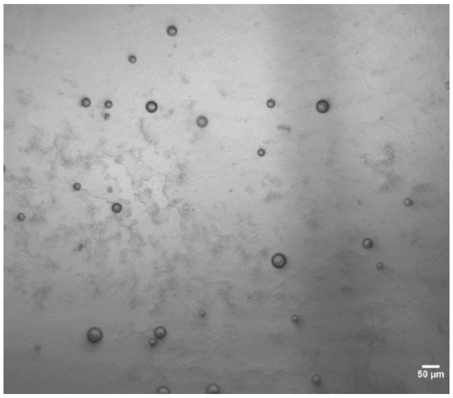

Figure 1: Spherical micro-droplets on the SH surface (scale bar: 50 µm).

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Role of Liquid-liquid Phase Separation in the Regulated Secretory Pathway

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Liquid-liquid phase separation (LLPS) is an emerging phenomenon in cell physiology and pathology, gaining significant attention in the last decade [1]. Biomolecular condensates, generated through the process of LLPS, play a crucial role in various cellular functionalities, such as cell signaling, transcription regulation, vesicular trafficking, and many more [2]. LLPS is also shown to be associated with aberrant liquid-to-solid phase transition which has implications in diverse pathogenesis, including neurodegeneration and cancer [3]. Amyloid aggregation is a pathogenic hallmark for neurodegenerative diseases as all the major disease-associated proteins such as α-Synuclein, Tau, Aβ, etc. are shown to form amyloid-rich inclusions in the diseased neuron [4]. However, amyloid fibrils can also be associated with cellular functionality, termed functional amyloid [5]. One such example of functional amyloid is peptide hormone storage in secretory granules in a regulated secretory pathway which releases native monomeric protein by regulated exocytosis [6]. The present work investigates the role of LLPS in the regulated secretory pathway during the storage and release of peptide hormones. The work highlights the intrinsic property of hormones to undergo phase separation in secretory-granule-relevant *in-vitro* and *in-cell* experimental conditions. Moreover, the work also shows that the environmental factors of the protein secretory pathway facilitate liquid-liquid phase separation and quick but reversible liquid-to-solid transition into amyloid-like assemblies which may have a direct impact on the storage and release process of hormones in the regulated secretory pathway.

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BM-P42

Conformational fluctuation can modulate the phase separation of yeast prion protein

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Intrinsically disordered proteins (IDPs) can undergo Liquid-liquid phase separation (LLPS) involving multivalent interactions between polypeptide chains. Yeast prion protein, Sup35, undergoes LLPS under macromolecular crowding. Crowding can significantly alter the phase separation ability of IDPs by changing the interaction forces involved in phase separation. Through a combination of Single-molecule techniques, computational tools, and other biophysical assays, we have demonstrated that the conformational fluctuations of Sup35 can regulate the phase separation of the protein. In a model crowded environment, it can adopt both expanded and compacted states. This conformational switch is influenced by the nature and threshold concentration of the crowder used. Furthermore, our findings reveal that distinct conformational states under various crowder concentrations can impact the LLPS of Sup35 in diverse ways. The extended conformation favors LLPS whereas the compacted one opposes LLPS. Consequently, this modulation influences the protein's aggregation propensity. This study underscores the importance of having sufficient "breathing space" for the protein to undergo LLPS within a crowded milieu.

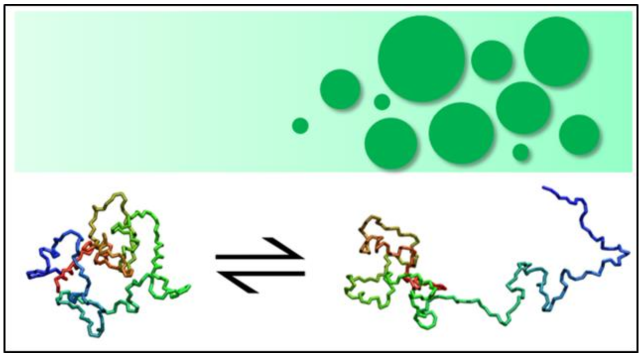

Fig. 1: Conformational guided phase separation of Sup35

Reference : Franzmann TM, et al. Science. 2018 Jan 5;359 (6371)

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Phase Separation of Intrinsically Disordered Proteins in Analytical and Field Theoretic Models

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Biological condensates are of fundamental biophysical and biomedical interest. Numerous experimental studies suggest that bio-condensates like nucleolus, stress-granules, p-bodies etc. are physically underpinned to a significant degree by liquid-liquid phase separation (LLPS) of intrinsically disordered proteins (IDPs) driven by amino acid sequence pattern dependent multivalent interactions of several types such as electrostatics, hydrophobicity, cation-Pi, Pi-Pi etc. Polymer field theories are needed to describe sequence dependent LLPS because mean field theories like Flory-Huggins theory can not fully account for sequence dependence. Using field theory models we have studied, sub-compartmentalization in phase separated droplets containing multiple IDPs, effect of inhomogeneous dielectric background on IDP phase separation, LLPS in chemically reactive environment and protein phase separation driven by non-electrostatic interactions incorporated through spectral decomposition of molecular dynamics force fields.

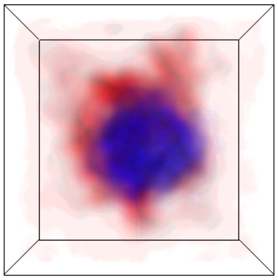

Figure 1: Field theoretic simulation density snapshot showing demixing of two IDPs, shown in red and blue, upon co-phase separation.

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BM-P45

Force measurements on cells and Near-field optical microscope platform

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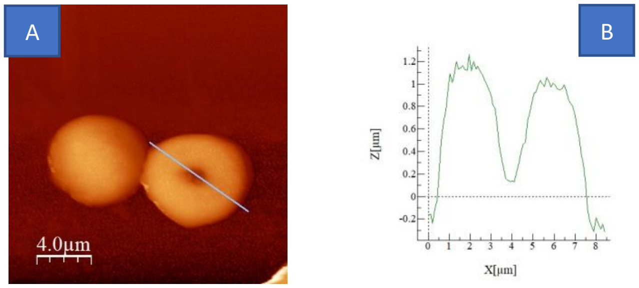
Our study focused on human Red Blood Cells (hRBCs) exposed to various physical and Chemical conditions. hRBCs can undergo large deformations when subjected to external forces, which allows them to pass through capillaries vessels that are narrower than the diameter of a resting RBC. The deformability of RBCs allows them to flow in smaller capillary vessels while transporting oxygen and carbon dioxide to body tissues. Here we studied the 2D and 3D physical properties of RBCs membrane using AFM. we are interested to stiffen the human RBCs cells at one small portion using functionalized AFM probe and characterize the Force and distance measurement and Young's modulus of the nanoscale portion. The structural morphology of red blood cells we studied in their own media(liquid) using atomic force microscopy (AFM) which is coupled with a Near field scanning microscope (NSOM). Atomic Force Microscopy (AFM) is a powerful tool for exploring the interaction between ligands and receptors, as well as their exact locations on the red cell surface. The red blood cells were diluted in phosphate buffer solution and immobilized on a poly l lysine-coated glass coverslip using a 2% concentration of glutaraldehyde. The shear force feedback AFM gives the morphology of the surface of the sample by sensing the surface line by line with a size 10nm tip. Here using this AFM technique, we do study the physical properties of red blood cells. And also, we are trying to study the elastic nature of the hRBCs using optical tweezers.



A. 2D AFM topographical image of RBCs, **B.** Height graph of image

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BM-P46

Rheological characterization of bacterial suspensions in plant mucilage

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Plant roots exude gelatinous polysaccharide substance termed as “root mucilage”. Rhizosphere is a soil layer of direct influence of root exudates, soil microbes and soil nutrients. The complex biochemical cycles and symbiotic relationship among these elements in rhizosphere makes it distinct from the bulk soil in different aspects such as mechanical response, water dynamics and nutrient uptake and plays a crucial role in plant ecology [1]. The exuded root mucilage acts as a rich carbon source for the soil microbiota and establishes a mutual relationship between microbes and root nodes [2]. Additionally it is shown that the motility of the microbes also affect the mechanical properties of the respective material system [3]. To study the interactions between microbes and mucilage is challenging and how the presence of microbes affect the rheological properties of mucilage is of research interest. Generally, the microbes are cultivated in a nutrient broth and growing bacteria in an unusual medium like seed mucilage is challenging. As an initial step, Bacillus subtilis, a soil microbe is successfully grown on chia seed mucilage which can be treated as ‘model root mucilage’. The growth kinetics of Bacillus subtilis in mucilage media is studied. Mucilage + bacterial suspensions and pectin + bacterial suspensions are prepared by suspending grown bacteria in higher concentrations. Steady shear and oscillatory shear rheological experiments are performed on these suspensions on a conventional rheometer. Change in viscoelastic properties of mucilage and pectin in presence of bacteria is studied and analyzed.

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Phase separation of p53 and its functional implications

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Transcription factor p53, regarded as the 'guardian of the genome,' comprises five major functional domains, consisting of multiple intrinsically disordered regions and a low-complexity region. Here, we show that p53 phase separates to form dynamic liquid-like condensates in vitro and in mammalian cells. Our data show a clear spatiotemporal regulation of these condensates inside cells and altered physical states with time. The liquid-to-arrested state transition of these condensates occurs in a nucleo-cytoplasmic localization-dependent manner. Nuclear condensates show a more liquid-like nature than cytoplasmic condensates. The state of these condensates is altered due to multiple genetic as well as environmental factors. Hotspot mutants of p53 (which are prevalent in cancer), the addition of stress, and the stabilization of p53 independently modulate the liquid-to-solid transition dynamics of these condensates. This study provides us with mechanistic insights into the modus operandi of p53 as a transcription factor

BM-P48

Molecular dynamics investigation of the dynamical response of the interfacial waters near DPPC bilayer to Hyaluronic acid

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Hyaluronic acid (HA) is a long, hydrophilic polyanion that aids in cellular contact, coating of cellular surfaces, and lubrication. It is overexpressed in cells and body fluids during pathogenic situations like colon cancer. Previous studies have shown that the interaction between HA and lipid molecules is mediated by water molecules. The dynamic properties of the interfacial waters are critical to understand spectroscopic data and the mechanical properties of the HA-lipid complexes. However, there is no report on the theoretical understanding of HA's significance in water dynamics near lipid vesicles. To that end, we take Dipalmitoylphosphatidylcholine (DPPC) lipid bilayer and HA of different sizes and concentrations in our fully atomistic molecular dynamics simulation. Our findings suggest that at the HA-DPPC bilayer interface, HA restricts the translational and rotational diffusion of the water molecules. We note the signature of heterogeneity in the dynamics of water. We explain our results based on the inherent hydrophilic nature and the network structure of HA molecules at the interface.

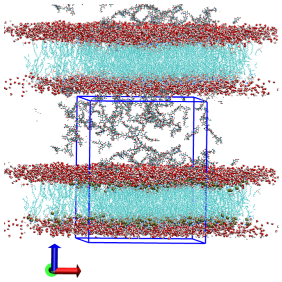

Figure 1: Model of the simulated system. Interfacial water molecules (red VDW representation) are shown along with HA(Licorice) and lipid bilayer (cyan Bonds).

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Title - Biomimicking Of The Natural Mucilage By Pectin-based System

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Pectin, a water-soluble polysaccharide that is usually found in the cell walls and intercellular tissues of certain plants. Depending on degrees of acetylation, methylation and contents of galacturonic acid in it, pectins demonstrate gelling properties and can form complexes with divalent ions like Ca2+ and Mg2+. The degree of methylation (DM), can be expressed as the ratio of methyl-esterified carboxyl groups to the total amount of galacturonic acid units and this is one of the crucial parameters related to gelling capability. It may be determined using infrared spectroscopy. Mucilage, a gelatinous substance produced by nearly all plants and the most important chemical component of mucilage is pectin. In plant physiology, this mucilage fulfils a variety of functions including adhesion, protection, lubrication, nutrient acquisition etc. which make it an area to study more. Hence, the idea of mimicking the natural mucilage came up by studying the response of pectin solution along with pectin gel system. The rheological properties of the pectin solution and pectin-Ca and pectin-Mg gels were investigated. The apparent viscosity and other rheological responses of the solutions and gels were directly related to the pectin concentration and stoichiometric ratio respectively. Pectin solution and pectin gel systems showed shear thinning behaviour. Rheology highlighted linear as well as non-linear mechanical responses and gel nature with possible contribution of egg box bundles by exploring large and small amplitude oscillatory shear experiments. These Egg-boxes are dimers, which are formed when two homogalacturonan segments are parallel and bridged together by divalent ions. These responses can be fitted well with various rheological models too.

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BM-P50

Mechanism of nucleation and liquid-to-solid transition for α-synuclein liquid-liquid phase separation

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Abstract:

Liquid-liquid phase separation (LLPS) and subsequent liquid-to-solid phase transition (LSPT) is an important bio-molecular phenomena for the formation of membraneless organelles as well as disease associated protein aggregation. Aggregation of natively unstructured α-synuclein has been shown to be associated with neurodegerative Parkinson's disease pathologically characterized by the formation of lewy bodies and lewy neuritis rich in α-synuclein aggregates, fibrils and other components such as metal ions, glycosaminoglycans and lipids. Recently it has been shown that LLPS is the possible nucleation mechanism for α-synuclein aggregation. But how liquid-to-solid transition is initiated inside a liquid droplet is still not clear. Further the effect of PD-related factors like metal ions, lipids, and glycosaminoglycans on phase separation has been studied but underlying mechanism is unknown. The aim of my research is to understand the mechanism of nucleation and liquid-to-solid transition for α-synuclein LLPS, solidification event of α-Synuclein droplets spatio-temporarily and the effect of PD-associated factors on α-synuclein LLPS.

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Decorating Filamentous Viruses: Design & Self-Organization of Virus based Colloidal Molecules

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Filamentous viruses have been widely studied for decades as model system of rod-shaped particles in soft condensed matter [1,2]. Their ability to tune precisely their interaction results in a very rich phase behavior with a myriad of liquid crystalline states [3,4]. In this talk, we will go beyond the use of viruses as raw colloidal particles by discussing recent advances in their functionlization to create more complex structures [5]. Different strategies of regio-selective functionlizations will be shown, in order to bind virus tip with either organic molecules such as fluorescent dyes [6,7], or with metallic nanoparticles [5]. The resulting hybrid nanostar morphoplogies will be presented, inlcuding their self-assembly properties as well as their dynamics probed at the single particle level.

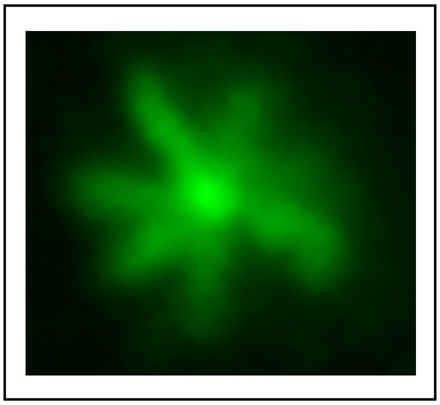

Figure 1: Hybrid nanostar particle formed by an Au core decorated with filamentous viruses acting as arms and observed by fluorescence microscopy. The length scale is given by the size of the virus arm of 1μm.

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CO-02

Coating Hydrophilic and Hydrophobic Iron Oxide Nanoparticles with Polymers using Novel Flash Nanoprecipitation Techniques.

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Magnetic monodomain iron oxide nanoparticles (IONPs) find wide biomedical applications ranging from diagnostics to therapeutics such as in magnetic hyperthermia, targeted drug delivery, etc.[1] Their performance in such applications is governed by their magnetic properties which in turn are influenced by particle size, shape, inter particle interactions among others. IONPs synthesized via thermal decomposition of iron – oleate,[2] pentacarbonyl,[3] etc in organic solvents leads to precise control of size, size distribution, magnetic properties when compared to IONPs synthesized via co-precipitation. However, for biomedical applications, these IONPs should be water dispersible - phase transfer also introduces other caveats such as aggregation, reduction in magnetic properties and so on. While water dispersibility is not a challenge for the co-precipitation IONPs, to tailor the particles towards specific applications, post functionalization is an important subsequent step.

Herein, we report for the first time, a novel flash nanoprecipitation (FNP) technique that has been tuned to both (i) functionalize IONPs synthesized via thermal decomposition whereby facilitating phase transfer and polymer encapsulation simultaneously and (ii) coat hydrophilic IONPs synthesized via co-precipitation via hydrophobic ion-pairing.

In the thermal decomposition of iron oleate, the oleic acid concentration, ramp rate, reflux time and solvent were optimized to yield IONPs with high magnetic saturation ~70 emu/g and small sizes (< 10nm) (particles synthesized in benzyl ether). The reaction conditions for FNP were optimized for bare polymeric NPs, following which, the synthesized IONPs were phase transferred by suspending in tetrahydro furan (THF) with Poly Lactic Glycolic Acid (PLGA) and allowing this solution to mix with an opposing stream inside a vortex mixer containing water with Tween 80 (stabilizer), which acts as a non-solvent. In case of hydrophilic IONPs, they were mixed with oleic acid surfactant and PLGA in THF to constitute the solvent phase. Our results show the formation of PLGA coated IONPs in both cases, with a hydrodynamic size in the range of 70 - 220 ± 10 nm and high colloidal stability, shown by high zeta potential -20 ± 5 mV, proving the versatility of FNP.

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Activity induced non-monotonic aggregation in a mixture of chemically active and passive particles

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Spontaneous symmetry breaking has been shown to be the genesis of self-assembly in a mixture of spherically symmetric chemically active and passive colloids, forming dense clusters [1,2]. We study the kinetics of such self-assembly, driven by the phoretic motion of passive colloids following the chemical gradient generated by the active seeds (Fig. 1). A non-monotonic effect of activity on aggregation is the key observation in our work. We rationalize such non-monotonicity in the clustering by the hybrid coarse-grained simulations. The average cluster population and the variation of their size as a function of time, the stability of clusters, and their dynamics are the key quantifications that help us comprehend the aggregation. The model offers the additional advantage of including explicit hydrodynamic interaction among the colloids, which is often neglected in such simulations. And it turned out that hydrodynamics has a significant role in colloidal self-assembly and can not be overlooked in chemically active systems [3].

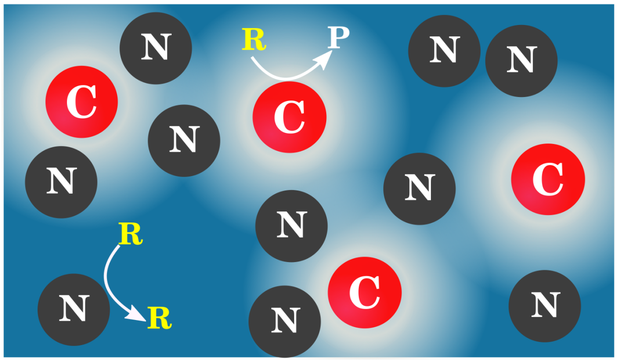

Figure 1: Schematic illustration of catalytic **C** (red) and non-catalytic **N** (grey) colloids dispersed in a solvent. **C** converts the **R** solvent to **P**, thus creating a uniform distribution of **P** around it (white color), whose value is maximum near the catalytic sphere's surface and decays radially outwards. Non-catalytic colloids can react to the concentration gradient created by active particles due to diffusiophoresis, and give rise to self-assembled dynamic structures.

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Indian Society of Rheology

Light-controlled patterning of metallic nanoparticles

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Vertical deposition is a conventional particle patterning technique to realize large-area patterning for photonic crystal [1] and electronic devices [2] applications. Though this method is exploited for achieving large-area patterning, inscribing patterns with desired dimensions over the substrate remains a challenge. Light-induced flow based patterning techniques are gaining increased attention as it allows real time and non-contact control over the patterning process [3,4]. Herein we demonstrate a technique for the precise patterning of Gold nanoparticles by the synergy of light-induced thermocapillary flow and vertical lifting method. The principle relies on the accumulation of particles near the contact line of the liquid meniscus in contact with a solid substrate due to light-induced thermocapillary flow and controlled lifting of the substrate out of the liquid, as shown in Figure 1a. We performed both simulation and experimental studies of the developed patterning technique. By modulating the lifting velocity, we could achieve different patterns, such as dots and lines (Figure 1b) with different morphology. Further, we demonstrated the applicability of the developed pattern to realize large-area patterning of microparticles.

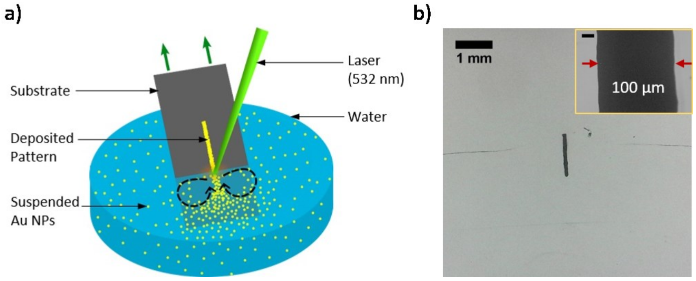

Figure 1: a) Schematic showing the principle of light-induced thermocapillary flow and vertical lifting driven patterning of Gold nanoparticles. b) Optical image of the line pattern (magnified microscopic image is shown in the inset). Scale bar in the microscopic image corresponds to 10 µm.

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Bioinspired structures via self-assembled of colloidal particles

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Colors from structures found in nature dependent on the size and periodic arrangement of nanostructure elements. Many birds and insects show photonic crystals structures. While few creatures such as chameleon and sapphirinid copepods have an ability of tuning photonic crystal's structure to produce a variety of colors. This has provided a guideline for unique geometry and corresponding structural color effects phenomenon. Micropatterning or structuring of solution-mediated materials is a fundamental requirement for desired high-performance functions of the materials in various applications. Traditionally microscale patterning not only boosted up the microelectronics industry but also allowed emergence of lab on a chip for low-cost analytical instrumentation in parallel. Especially, nanoscale feature size opened new opportunities by offering many advantageous chemical, optical, electrical, and thermal characteristics derived from their high surface to volume ratio. In this reason, it is highly demanding for developing effective methods which is not only simple and low-cost but also is less limited in dimension, complex structure, and even 3-D patterns and/or structures. Several fabrication methods have been developed. Comparing with other techniques, such as lithographic, nanoimprinting, and microcontact printing, printing is a direct depositing technique using the liquid phase materials. By virtue of its cost effective, easy to handle and speediness, printing technique has become a reliable technique for high quality and well pattern fabrication.[1] However, it is still difficult to obtain desired morphologies by printing technique. The proposed research is to develop an inexpensive micropatterning platform using microsyringe pump as illustrated in Figure 1a. Furthermore, to understand the basic underlying mechanism of color exhibits from nanostructure of the self-assembly of particles on the glass substrate as shown in Figure 1b.

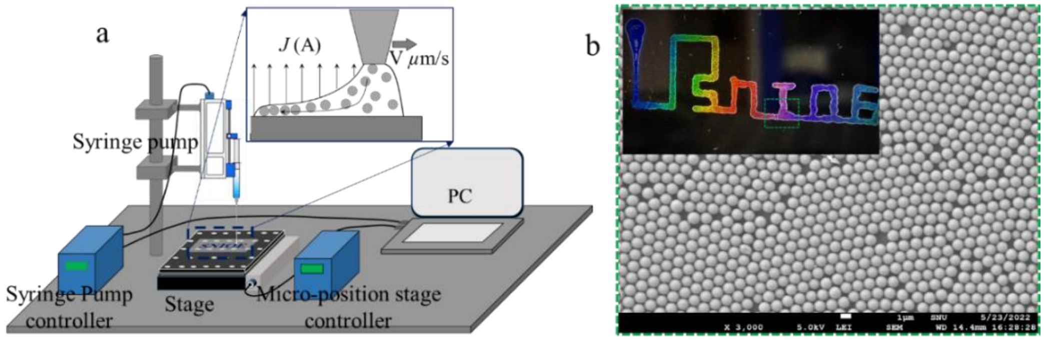

Figure 1. a. Illustration of micro-nanopatterning using microsyringe pump; b. The black and white logo 'SNIOE' produces iridescent photonic crystals pattern due to self-assembled of the particles and the corresponding SEM image.

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Indian Society of Rheology

Pe dependent pair interactions in self-propelled droplets

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Pair-interactions of active oil (5CB) droplets, propelled using micellar solubilization mechanism, were explored in quasi 2D confinement at varying Péclet numbers (Pe). Using PEO of high molecular weight as macromolecular additive to the aqueous surfactant solution (continuous media), self-propelled motion with Pe was achieved. In these systems, the droplets exhibit a unique unfriendly scattering behavior (figure 1(a-b)), wherein droplets repel each other on approach. This scattering phenomenon is attributed to the repulsive chemical field interactions originating from the accumulation of the filled micelles which are known as poison for the droplet motion [1]. The repulsive chemical interactions outweigh the attractive hydrodynamic interactions expected to result from the puller swimming mode [2]. In absence of PEO as additive, the associated Pe was higher. In such cases, the influence of the chemical field was found to be significantly lower and depending on the approach orientation, droplets are hydrodynamically attracted to each other (figure 1(c)) [2]. They display intriguing coupled-motion such as side-by-side cruising, offset tandem and tandem. Overall, this study highlights the significant influence of both hydrodynamic and chemical fields on active droplet dynamics during pair-wise interactions across different Pe. We believe that the valuable insights gained from the study will contribute to a deeper understanding of multibody interactions within active droplet systems.

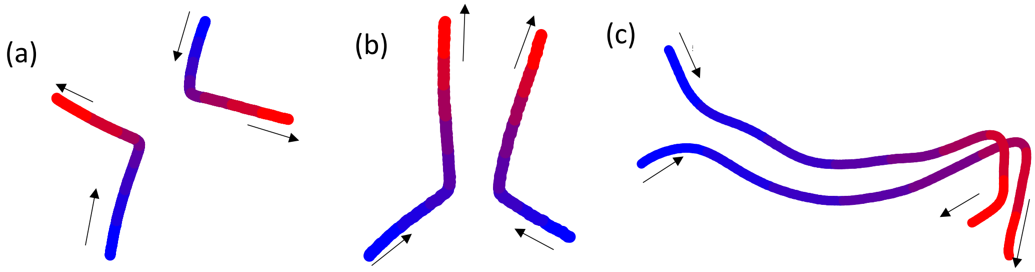

Figure 1: (a-b) Representative trajectories of active droplets involved in binary-interactions in PEO (Polyethylene oxide 8000 kDa molecular weight) aqueous TTAB surfactant solution. (c) Representative trajectory of droplet pairwise interactions in just aqueous TTAB surfactant solution.

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Hybrid Metamaterials with Controllable Twist

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Chirality is a geometrical property described by continuous mathematical functions. However, in chemical disciplines chirality is often treated as a binary left/right characteristic of molecules rather than a continuity of chiral shapes. While being theoretically possible, a family of stable chemical structures with the same shape and progressively tunable chirality is yet unknown. Here we present such structures in the form of nanostructured microparticles with anisotropic bowtie shape and widely tunable twist angle, pitch, size, thickness, and length. The self-limited assembly of the bowties made from cadmium and cystine enables high synthetic reproducibility, size monodispersity, and computational predictability of their geometries for different assembly conditions (Fig. 1). The bowties nanoassemblies display multiple strong circular dichroism peaks originating from absorptive and scattering phenomena. Unlike classical chiral molecules, these particles display a continuum of chirality measures that correlate exponentially with the spectral positions of the circular dichroism peaks. Bowtie particles with variable polarization rotation were used to print photonically active metasurfaces with spectrally tunable positive/negative polarization signatures for light detection and ranging (LIDAR) devices.[1]

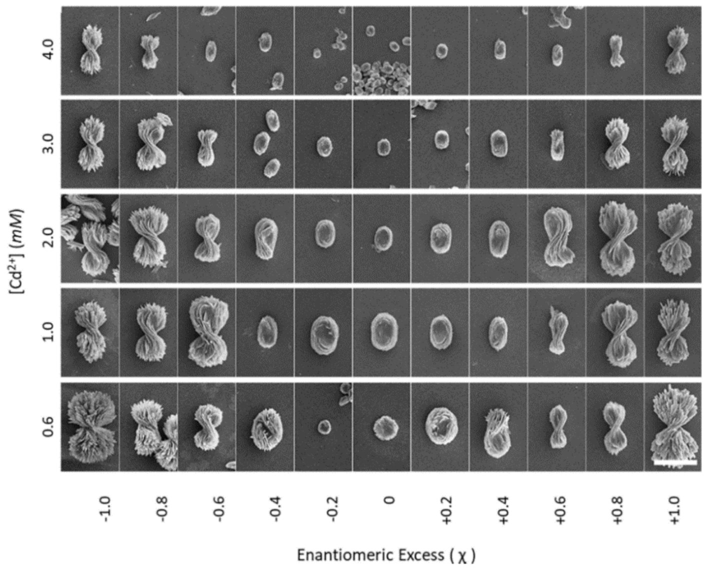

Figure 1: Phase diagram of different bowtie shapes made by changing the ratio of cadmium ions to cystine ions and the enantiomeric excess. SEM images show variation in twist and size controlled by the nanoscale interactions varied independently along the two axes of the phase diagram. The scale bar is 5 µm.

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Indian Society of Rheology

Opto-thermoelectric trapping of fluorescent nanodiamonds

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The unique properties of fluorescent nanodiamonds, such as small size, stability and biocompatibility make them a promising material for sensing and biomedical imaging applications [1-2]. But in order to expand their potential use for single spin imaging and optically detected magnetic imaging, their precise control in solutions is crucial. However, optical tweezers are insufficient in trapping nanoparticles as they are subject to stronger thermal fluctuations due to very small size and mass. Opto-thermal trapping techniques and in particular the opto-thermoelectric trapping has emerged as a promising technique for such applications [3].

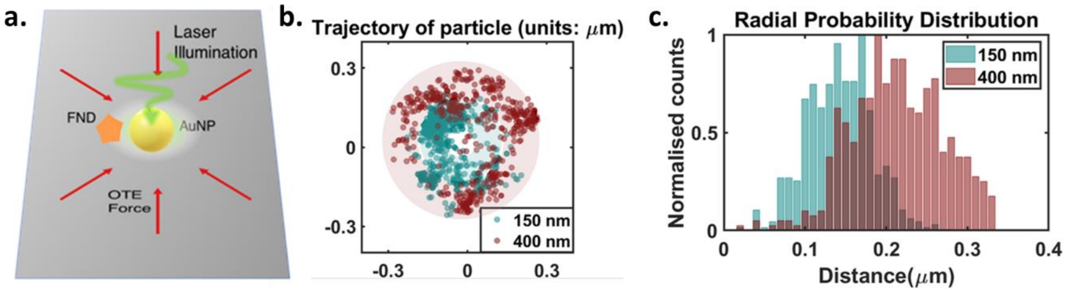

Figure 1. a) Schematic of plasmon-assisted Opto-thermoelectric trapping of fluorescent nanodiamonds on Gold Nanoparticles. The surfactant (CTAC) facilitates an electric field which attracts the FND to AuNP. b) Trajectories of trapped FND using 150 and 400-nm diameter AuNPs. c) Corresponding radial probability distribution.

We have shown how chemically-prepared gold nanoparticles and silver nanowires can facilitate opto-thermoelectric force to trap individual entities of FNDs using a long working distance lens, low power-density illumination (532nm laser, 12 $\mu W/\mu m^2$) [4]. Our trapping configuration combines the thermoplasmonic fields generated by individual plasmonic nanoparticles and the opto-thermoelectric effect facilitated by the surfactant to realize a nano-optical trap down to a single FND 120 nm in diameter. We utilize the same trapping excitation source to capture the spectral signatures of single FNDs and track their position. By tracking the FND, we observe the differences in the dynamics of FND around different plasmonic structures. We envisage that our drop-casting platform can be extrapolated to perform targeted, low-power trapping, manipulation, and multimodal imaging of FNDs inside biological systems such as cells.

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Indian Society of Rheology

Solution Processing of Low-dimensional Materials and Applications

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Low-dimensional Materials like graphene, transition metal dichalcogenides, h-BN, transition metal oxides and layered double hydroxides possess the potential for applications across various fields. Liquid phase exfoliation of these layered crystals enables the solution processing of dispersions of mono- and few-layers, and provides a scalable viable alternative to other physical and chemical routes. The quality of the dispersions and their applicability are dependent on the exfoliation and stabilization of the exfoliated material by the solvent, often chosen on the basis of Hansen solubility parameters (HSP). In this work, the factors at play in liquid phase exfoliation besides HSP are explored via various experimental methods, in order to further enhance the versatility of the process by providing a deeper insight. By considering molecular aspects of the solvents, highly concentrated nanosheet dispersions were obtained in a low boiling point solvent. I will also discuss about experimental determination of the HSP of layered materials. I will be concluding my talk by discussing some of our recent efforts in exfoliating non-layered materials and applications of the 2D dispersions in various fields like flexible electronics, energy storage/conversion devices and electrochemical biosensors.

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The Impact of Surface Ligands in Regulating Nanoparticle Chemistry

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The underlying power of interplay of forces [1] in controlling the properties and functions at the nanoscale will be highlighted in the presentation. This interplay was achieved by installing attractive and repulsive forces, via proper ligand chemistry, which will guide the nanomaterials to interact with their surroundings as per the need. Along with improving the existing properties, the balancing of attractive and repulsive forces holds the prospects of imparting newer functions as well. The concept of 'ligand-directed interplay of forces' is extensively practiced by our group for addressing many challenges in the areas of self-assembly, catalysis, and light harvesting.[2] The journey has been rewarding so far in terms of achieving many important feats in nanoscience, such as self-assembly under equilibrium and nonequilibrium regimes,[3] outplaying ligand poisoning in catalysis,[4] and channelizing the flow of energy and electron in donor–acceptor systems[5]. These advancements accomplished through the fine-control over interparticle interactions are expected to expand the scope of nanomaterials in energy research.

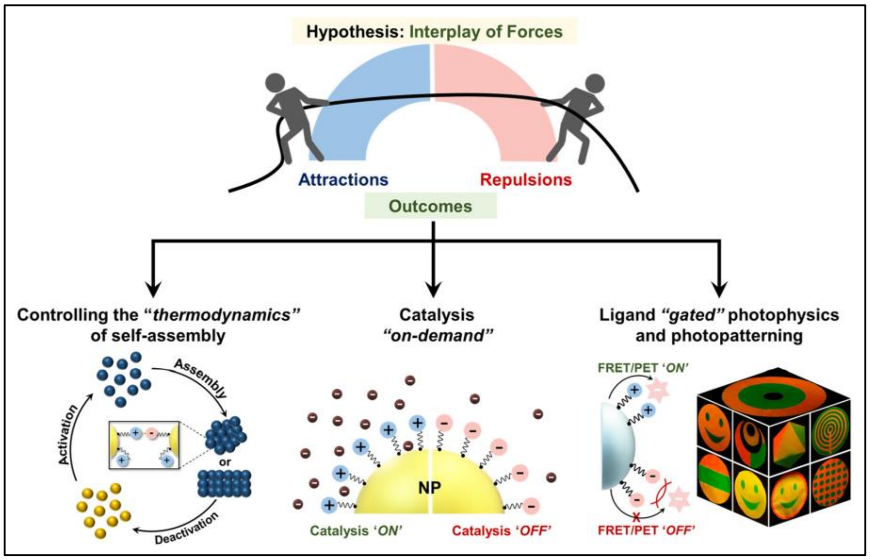

Figure 1: Schematics showing the impact of 'ligand-directed interplay of forces' in achieving some of the desirable feats in self-assembly, (photo)catalysis and photophysics at the nanoscale.

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Engineering Polymers and Colloidal Particles to Control and Tailor Crystal Habit

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Particle shape has a bearing on physicochemical properties such as rate of dissolution, perceived colour (in the case of pigments), packing density and flowability in the case of powders, and rheological characteristics of wet and dry suspensions. Growth modifying additives have been long used to control the shape of particles formed during crystallization. Growth modification by the use of small molecules and salts dissolved in the mother liquor is relatively well understood. However, the growth modifying function of larger molecules such as polymers and polymeric surfactants is not as well understood.

Using bright-field optical and fluorescent confocal microscopy, we study the microstructure of polycrystalline wax suspension crystallized from oils containing different growth modifiers and at varying concentrations. Here, we demonstrate that similar hierarchical crystal habits can be achieved from the use of modifiers that span a range of lengths scales: molecules (< 2 nm), polymers (~5-10 nm), and colloidal particles (< 1000 nm). We also demonstrate the subsequent effect of the hierarchical crystal habits, quantified in terms of network connectivity and particle dimensions, on the rheological behaviour of these suspensions. The similarity of observations for the wide range of additives and their respective growth mechanisms will be discussed.

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CO-P1

Role of Softness on transition temperatures for PNIPAM Microgels

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PNIPAM microgel particles are well-known due to their ability to undergo reversible volume phase transition. Anionic PNIPAM microgel particles of different softness (by varying crosslinking density during synthesis) were synthesized by surfactant free emulsion polymerization (SFEP) [1]. It has been already reported that there is a variation in transition temperatures of size, namely volume phase transition temperature VPTT and electrophoretic mobility, namely electrokinetic transition temperature ETT [2]. In this study the effect of softness on VPTT and ETT, will be analyzed by measuring particle size and electrophoretic mobility at different temperatures. A hypothesis that provides physical insights into the transition temperatures and the effect of softness on this transition temperature will be put forward. Finally, a cationic polyelectrolyte will be mixed with these anionic microgels to form the coacervates (soft nanocomposite) to study the effect of the inter particle potential for nanocomposite formation.

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CO-P4

Bulk nanobubble generation by gas supersaturation method

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For the past decade, nanobubbles have been shown to have numerous applications due to their unique properties. Despite its potential in enhancing gas-liquid operations, limited to no studies have been conducted on nanobubble generation in pure organic solvents with strong scientific evidence [1]. Furthermore, there is no direct evidence that explains the generation of nanobubbles by gas supersaturation mechanism. Since there is a strong dependence of gas solubility over temperature, therefore, a solvent at a high temperature, when, mixed with the same solvent at a low temperature releases the excess gas that may nucleate to form nanobubbles. The nanobubble generation was carried out with the variation in the temperature difference between hot and cold solvents ranging from 10˚C to 80˚C in the alcohols i.e., butanol, propanol, ethanol, methanol, and water. The nanobubbles are characterized by NTA (Nanoparticle Tracking Analysis) and DLS (Dynamic Light Scattering) in terms of bubble diameter, population and zeta potential. The results reported the formation of nanobubbles to be higher with maximum concentration in the range of 7.78×10^8 bubbles/mL at ΔT = 50-60˚ C. The zeta potential in water, methanol, and ethanol was observed to be negative while it shifted toward positive for propanol and butanol. The refractive index value calculation using Mie scattering theory confirmed the existence of nanobubbles as the values for all samples were close to unity (RI for air =1).

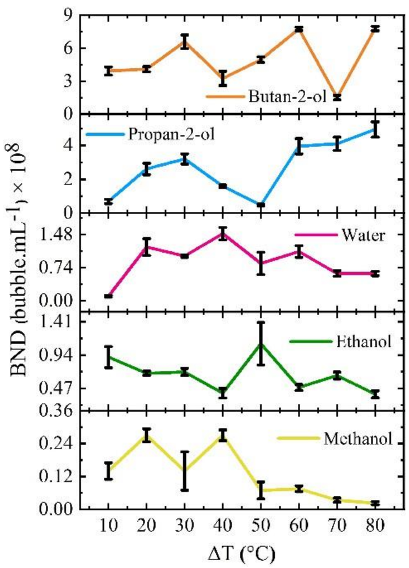

Figure 1: Bulk air nanobubbles concentration at different values of ΔT.

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Electric Field Induced Self Assembly of Polystyrene Spheres

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Self Assembly has been observed at all length scales [1], offering tremendous potential in the design of novel materials and micro-robotics. Colloidal self assembly has been studied under various conditions like capillary forces, depletion interactions, charge induced, field based interactions [2,3,4], etc. Electric field induced colloidal self assembly in particular, has garnered significant interest over the last three decades owing to its diverse applications in industry, including electro-wetting, particle sorting, and manipulation to name a few. We carried out a systematic investigation of the type of structure formations of micron sized colloidal particles under AC electric fields with varying frequency and amplitude ranges. We also studied the effect of changing the salt concentration, particle concentration and particle size on the assembled structures. Interestingly, non-close packed crystal formation was observed at lower frequencies and lower sizes while columnar stacking of particles was observed at higher frequencies and higher sizes. In the crystal formation, the packing density appears to vary with frequency range as well as the salt concentration due to a subtle interplay between different particle-particle and particle-substrate interactions. Tunable structures can therefore be achieved by varying any of these parameters for applications in a wide variety of technological domains.

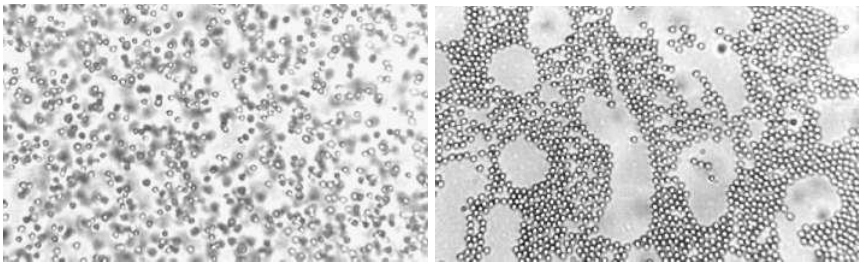

Figure 1: Polystyrene spheres of 1 µm diameter without electric field (left) and after the application of electric field (right).

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Field Induced Self Assembly of Anisotropic Particles

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Field-induced self-assembly of colloidal particles has become an exciting area of research due to its applications in materials design, nanotechnology, micro-robotics and biology. Electric and magnetic fields have been used to control the arrangement of colloidal particles into desired configurations for use as controllable microbots in applications such as targeted drug delivery. This has been extensively studied with spherical particles [1,2]. We extend this study to anisotropic particles with different geometries. We synthesize peanut-shaped and pseudocubic hematite (Fe_2O_3) particles by a sol-gel method [2]. They are then subjected to AC electric fields (out of plane) and magnetic fields (in-plane and out of plane) separately, as well as crossed electric and magnetic fields, and their assembly is studied systematically. Under an applied electric field, the long axis of the peanut-shaped particles gets aligned along the direction of the field, while the peanuts form chains along their short axis under an applied in-plane magnetic field. In crossed electric and magnetic field experiments, the electric field is utilized to orient the peanuts in an upright configuration with respect to the horizontal plane. This is followed by the application of a magnetic field on these upright particles, yielding switchable assembly and controlled motion. Our system shows promising potential for use as controllable propellers in microbots.

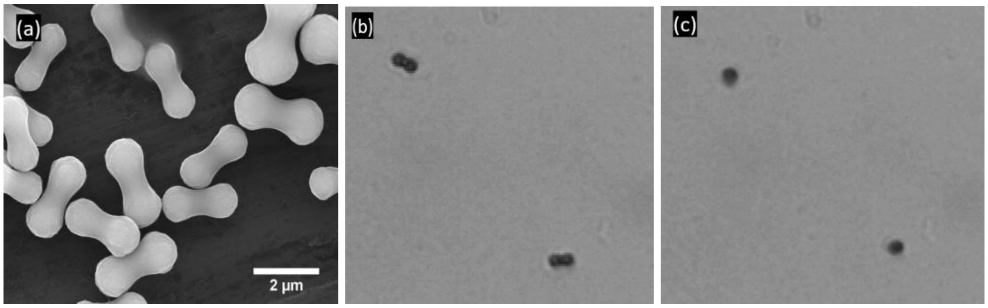

Figure 1: Peanut-shaped hematite particles (a) without any field lies on the horizontal plane (b), while under an AC electric field, their long axis orients perpendicular to the plane (c).

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CO-P9

Development of Antibacterial Waterborne Polymeric Coatings using Iodine Complex

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Despite the advancements in architectural coatings, the demand for antimicrobial coatings in this sector has increased significantly [1]. The COVID-19 pandemic was also a primary tool for an increase in demand, and production of antimicrobial coatings [2]. Typically, antimicrobial coatings are used to resist and decolonize microbial attacks viz. Biofilm formation, fungal contamination, black mold formation etc. [3]. In this study, we aimed to synthesize a water-based antimicrobial polymer nanocomposite, I-P(MMA/BA) by blending an iodine complex with a copolymer of poly (methyl methacrylate- butyl acrylate) latex with the aid of polyol and polyvinyl pyrrolidone. The antimicrobial efficacy was evaluated in two habitats viz. Planktonic and Biofilm. The biomass studies indicated that iodinated latex nanocomposite and film show excellent antibacterial and antibiofilm activity. About 85-97 % of biofilm formation was reduced by covering 15-30 % of an area with iodinated latex film respectively (Figure 1a). The contact angle measurement provides evidence for the good hydrophobicity that renders the stagnation of water over the surface (Figure 1b). Altogether, the dual functional water-based iodinated coating would display great potential in inhibiting biofilm formation on the surface of walls upon implementing the nanocomposite as the binder in paints.

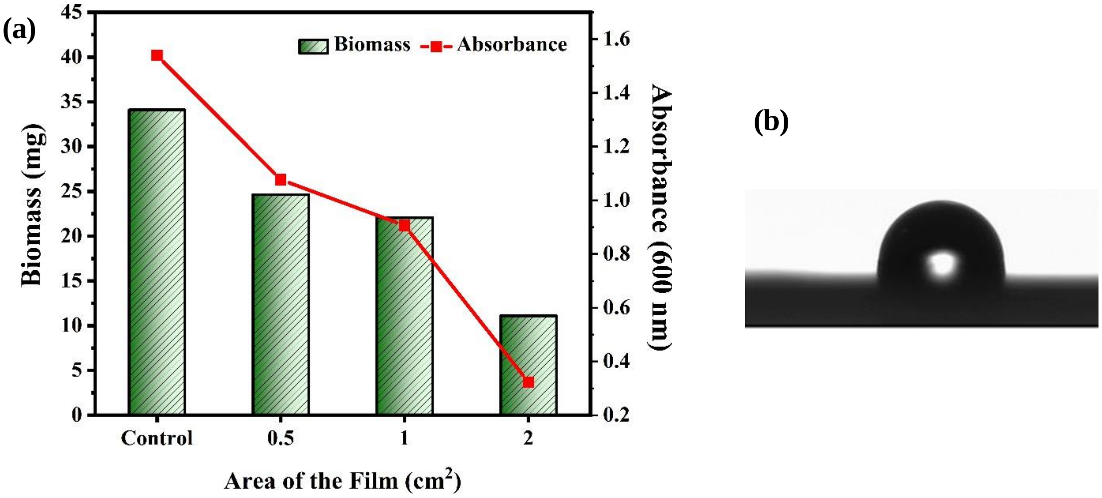

Figure 1a: Biomass (mg) and absorbance values for control (Blank) and films of areas 0.5, 1, and 2 cm^2. **Figure1b:** Contact angle measurement of the slide coated with iodinated latex.

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CO-P10

Understanding the effect of Methyl group of molecules in polymer solutions

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In the past decade, the effect methyl group on drug molecules has gained raising interests in medicinal chemistry. Recent research shows that, presence of methyl group enhances the pharmaceutical patency and specificity of the drugs and this effect is commonly known as the magic methyl effect. According to the literature, almost 70% of the commonly used drugs have one or more methyl groups present in it. Adding methyl group modifies many properties which are enhancing the half-life of the drug, increasing solubility, conformation effect, and boosting potency of a drug molecule. In this work we present an enhanced transport property of methylated molecules compared to non-methylated molecules in the presence of aqueous solution of polymer (polyethylene oxide). We demonstrate that the increase in diffusivity comes from the hydrophobic effect of the methyl group present in rhodamine 6G (R6G). To compare our results, we have taken homologs of R6G which is 6-HEX, and observed that the diffusivity of such molecules has much less diffusivity than the R6G molecule. We also seen the number of hydrogen bonds in 6-HEX is higher as compared to the R6G molecule. These results explain how the presence of methyl groups increases the diffusivity of small molecules in a semi-dilute polymer solution. This observation we have validated by using experiments with FCS, Molecular dynamic simulation with GROMACS, and scaling theory.

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Direction-dependent Dynamics of Colloidal Particle Pairs and the Stokes-Einstein Relation in Quasi-Two-Dimensional Fluids

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Hydrodynamic interactions are important for diverse fluids especially those with low Reynold's number such as microbial and particle laden suspensions, and proteins diffusing in membranes. Unfortunately, while far-field interactions are well understood in two and three dimensions, near-field interactions remain a challenge, limiting our comprehension of dense fluid suspensions. Here, we experimentally investigate hydrodynamic correlations between particles in quasi-two-dimensional colloidal fluids in the near-field. Surprisingly, we observe direction-dependent dynamics in particle pairs' displacement and relaxation in the body frame, quantitatively linked with measured near-field hydrodynamic interactions. This reveals a mechanism for the breakdown of the Stokes-Einstein relation (SER), which we observe and find to be less pronounced in directions with weaker hydrodynamic correlations. In total, the work uncovers significant ramifications of near-field hydrodynamics on transport and dynamic restructuring of fluids in two-dimensions.

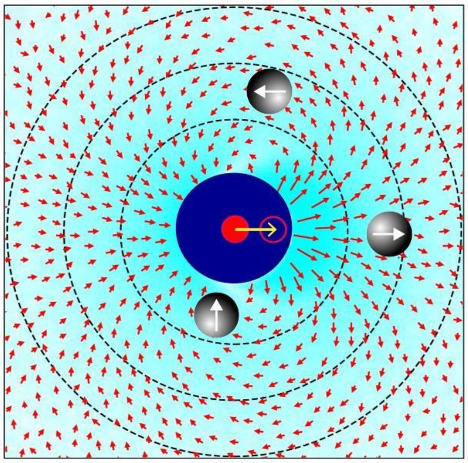

Figure 1: Polar colormap, $r(r,\theta)$, of hydrodynamic displacement field when the colloid at origin (solid red circle) moves towards the right (open red circle). The dashed radial circles represent r = $\{2,3,4\}\sigma$, σ is the particle diameter . Representative red arrows, with their head and length represent the direction and strength, respectively, of the field.

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Work distribution of a colloid in an elongational flow field and under Ornstein-Uhlenbeck noise

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The study of thermodynamic properties of microscopic systems, such as a colloid in a fluid, has been of great interest to researchers since the discovery of the fluctuation theorem and associated laws of stochastic thermodynamics. However, most of these studies confine themselves to systems where effective fluctuations acting on the colloid are in the form of delta-correlated Gaussian White Noise (GWN). In this study, instead, we look into the work distribution function when a colloid trapped in a harmonic potential moves from one position to another in a fluid medium with an elongational flow field where the effective fluctuations are given by the Ornstein-Uhlenbeck (OU) noise, a type of coloured noise. We use path integrals to calculate this distribution function and compare and contrast its properties to the case with GWN. We find that the work distribution function turns out to be non-Gaussian as a result of the elongational flow field, but continues to obey the fluctuation theorem in both types of noise [1]. A similar non-Gaussian behaviour in the work distribution was earlier reported, in which GWN was considered [2]. Further, the distribution starts out as asymmetric but becomes symmetric with time and reaches a non-equilibrium steady state. Finally, we also look into the effects of the various system parameters on the behaviour of work fluctuations and find that although the distribution tends to broaden with increasing noise intensity, increased correlation in fluctuations acts to oppose this effect. This study, therefore, is a step towards gaining a better understanding of the thermodynamic properties of colloidal systems under non-linear complex flows that also display correlated fluctuations.

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CO-P19

Optothermal Chiral Rotation in a Trap

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Since the pioneering discovery of optical tweezers by Arthur Ashkin [1], optical fields are being extensively used for the manipulation of micro and nanoscopic objects [2], non-equilibrium transport phenomena [3], and bio-medical applications [4]. Besides, optical fields can also induce thermal fields, leading to various interesting phenomena like self-assembly [5] and pattern formation, active dynamics [6], etc. This platform is also extensively used to induce and study the translational and rotational dynamics of microscopic colloidal structures for different microscopic mechanical applications. In view of the rotational dynamics, the protocol is divided into two distinct classes. Firstly, by direct transfer of angular momentum from the optical field itself [7]. Secondly, using the optical beam that does not possess any angular momentum. In this case, the rotation is achieved due to the asymmetric radiation force of the optical beam on the helically asymmetric structures [8].

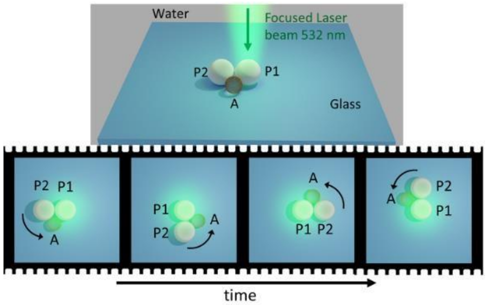

Figure 1: The schematic of the experiment shows an active trimer (AT) composed of two passive colloids (P1 and P2), and one thermally active colloid (A) exhibiting rotation under optical illumination of a 532 nm laser beam, where the black arrow indicates the direction of rotation.

In this work, we have experimentally demonstrated the emergence of optothermal field-facilitated chiral rotation in multi-component colloidal structures, composed of a binary colloidal mixture in aqueous suspension. The emergence of rotation can be understood from the asymmetric heating-mediated local optothermal force imbalance. The rotational dynamics can be modulated by the intensity of incident optical fields as well as the relative position of constituent colloidal entities. This study can potentially be useful to understand microscopic nonequilibrium thermodynamic systems and can be harnessed as a microscopic engine.

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CO-P20

Optical and Optothermal forces on Colloids in Evanescently generated Plasmofluidic Field

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Optical tweezers have emerged as a powerful tool to manipulate and study the physics of micro and nano-particles ever since its first demonstration by Ashkin et al [1]. Over time, the inability of conventional optical tweezers to manipulate very small objects due to their diffraction limited laser spot and high laser power necessity, has led to a need to develop alternate trapping techniques. One of the major advancements has come in the form of nano-optical tweezers which make use of surface plasmon resonances [2]. Surface plasmons (SP) are resonant oscillations of the surface electrons with the incident EM field and are evanescent waves that propagate along the metal surface. The two major advantages offered by SP are that evanescent fields can be confined beyond their diffraction limit and SP can couple with the EM wave to give highly intense localized optical fields called hot spots i.e. potential trapping sites.

In this work, we study the trapping mechanism of plasmofluidic traps, formed by coupling plasmonic trapping with thermally-induced fluid flow, to create colloidal assemblies [3]. Plasmonic trapping sites are generated by SP created on a metal film using total-internal reflection based Kretschmann geometry. The interplay between radiative (intensity gradient) and non-radiative (temperature gradient-induced fluid flow) effects of SP leads to large-scale nanoparticle assemblies of metallic and dielectric colloids [4]. The temperature gradient creates a convective fluid flow, driving nanoparticles afar to heated SP excitation spots. Once at the excitation spot, the optical force due to SP holds them against the upward fluid flow, forming a plasmofluidic trap. However, these temperature gradients, and resultant fluid flow, can be tweaked using the fluid column height and the polarization of excitation laser. The intensity of SP can be varied between minimum and maximum by switching between s- and p-polarized light respectively, thus enabling control over consequent temperature distribution and optothermal effects. The compactness of the colloidal assemblies can be controlled in thin fluid columns using the incident power, where at a threshold power, nature of assemblies formed by s- and p-polarized light reverses. Also, if two SP excitation spots are in vicinity, SP fields can interfere to give additional optical potential wells and temperature gradients, facilitating interesting colloidal assembly patterns under dynamic equilibrium [5]. Through this study, we explore various parameters which enable precise manipulation of nanoparticles as well as lead to a better understanding of the plasmonic and optothermal fields at play.

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Electrostatic self-assembly of GO-CNT nano-hybrid structures

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Carbon-based hybrid nanostructures consisting of graphene oxide (GO) and carbon nanotubes (CNT) could potentially provide superior properties relative to their individual components for mechanical and electrical aplications. However, the fabrication of such nanostructures at this length scale is found to be an arduous task, due to restacking of GO sheets and aggregation of CNTs. In this study, we report a scalable approach to develop highly ordered CNT intercalated GO hybrid nanostructures in an aqueous medium with electrostatic self-assembly process. The GO-CNT hybrids were synthesized by first modifying the GO and CNT with Poly(diallyldimethylammonium chloride) (PDDA) and Poly(styrene sulfonate) (PSS) via non-covalent interactions, resulting in highly stable dispersions of mGO, and mCNT respectively. The hybrid nanostructures were synthesized by homogeneous mixing of mGO and mCNT constituents with varying volumetric ratios. The hybrid nanostructures were characterized by zeta potential, dynamic light scattering, scanning electron microscopy (SEM), and transmission electron microscopy (TEM). From SEM the hybrid nanostructure with 1:0.5 mGO:mCNT (v/v) ratio was found with highly organized stacking of CNT intercalated GO sheets , owning to the charge neutralization point of the dispersion. TEM micrographs also show homogeneous distribution of CNTs on the GO sheets. Strengthened electrostatic interaction on the GO and CNT with polyelectrolytes prevents restacking and aggregation of GO sheets and CNTs; which further facilitates the self-assembly of oppositely charged nanoparticles into the formation of layered hybrid nanostructures. The proposed process provides a unique pathway in the large-scale production of GO-CNT hybrid nanostructures for membrane and high surface area applications in aqueous media.

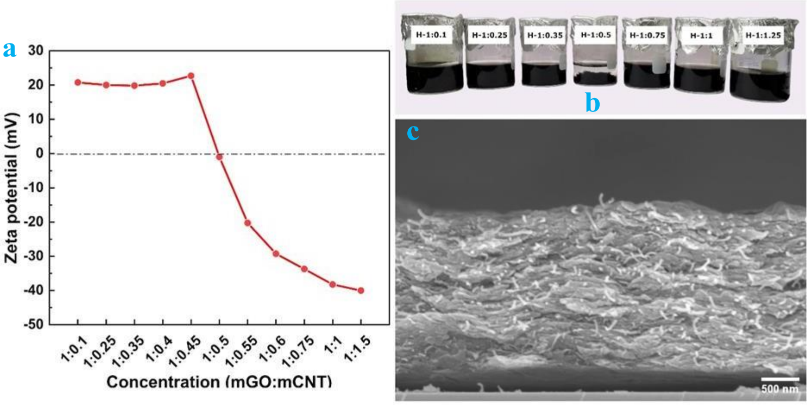

Figure 1: Change in zeta potential with addition of mCNT in mGO, (b) dispersion snapshots, (c) Cross-sectional SEM image of formulated GO/CNT hybrids with CNTs extruding out of GO sheets at 1:0.5 mGO:mCNT(v/v) ratio

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CO-P22

Long Range Electrostatic Screening in Zwitterionic Liquids

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As per classical electrolyte theories, the interaction energy in dilute electrolytes decays exponentially with distance, and the thickness of the electrical double layer increases with increasing counter-ion size and decrease in bulk ion concentration. But recent studies suggested that concentrated electrolytes exhibit a larger range of electrostatic repulsions between two charged colloidal particles than the Debye length [1], and a smaller screening length is associated with increasing ion concentrations [2]. The under-screening effect is inconsistent with the Poisson-Boltzmann theory and classical correlation models for Coulomb fluids [3,4]. A significant double layer expansion may be observed when standard electrolytes are taken at very high concentrations or salts having large ionic size asymmetries or diffusivities (e.g., ionic liquids). Using a combination of impedance spectroscopy and molecular dynamics simulations, we examine the interaction between two planar charged surfaces across ion asymmetric electrolytes to gain a deeper understanding of particle-particle interactions and dielectric dispersion of these suspensions. Furthermore, we discussed how the presence of these size asymmetric buffers affects the polarization of charge around the particle as well as the effect of their structures, which result in a permanent dipole when pH increases.

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Critical cracking thickness of mixed particles suspension film

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It is well known that drying films of colloidal suspensions such as wet clays, paints, and coatings may crack [1-6]. The thickness of maximum crack-free film depends on the size of particles, hardness, and nature of particle packing. Capillary pressure generated during drying is responsible for film cracking. Singh and Tirumkudulu [6], derived an expression for maximum crack-free thickness and experimented with different sizes of particles, demonstrating close agreement between theory and measurements.

Here, we identify the change in maximum crack-free film thickness when mixing soft particles in hard particle suspensions. We experimented with 0.5 µm silica (hard) and polystyrene (soft) particle suspensions and suspensions mixed in different volume fractions. A 5 µL droplet of mixed particle suspension was deposited on a clean glass substrate and left for drying in a vacuum oven chamber at 25 °C and 500 mmHg vacuum. The dried film had high thickness at the edges in comparison to the center region of the film due to the coffee ring effect [2-3] causing multiple cracks at the edges because of high stress in areas of high thickness. The cracks in the dried film were observed under a microscope. The film thickness was determined using a profilometer, which allowed determination of the maximum crack-free thickness. The effective shear modulus of mixed particle film was extracted from theory [6] by substituting the measured maximum critical crack-free thickness of the film. The extracted effective shear modulus of the packing was compared well with the lower bound shear modulus obtained from the rule of mixtures.

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CO-P24

Effective one-component theory for colloidal suspensions

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The theory delves into interactions within colloidal suspensions, focusing on solvent effects via a density functional approach. We establish functionals linking solvent-induced interactions to colloid density and solvent correlations. These interactions' nature, strength, and range hinge on solvent thermodynamics. We derive their contribution to the free energy functional and develop a self-consistent method for assessing colloidal particle interactions and correlations. Applied to hard-sphere mixtures, our findings reveal non-monotonic attraction trends with colloid packing, along with intensified repulsive peaks. Our theory explains complex dependencies of packing and size ratios on colloidal interactions, emphasizing the role of many-body effects in shaping colloidal suspension behavior.

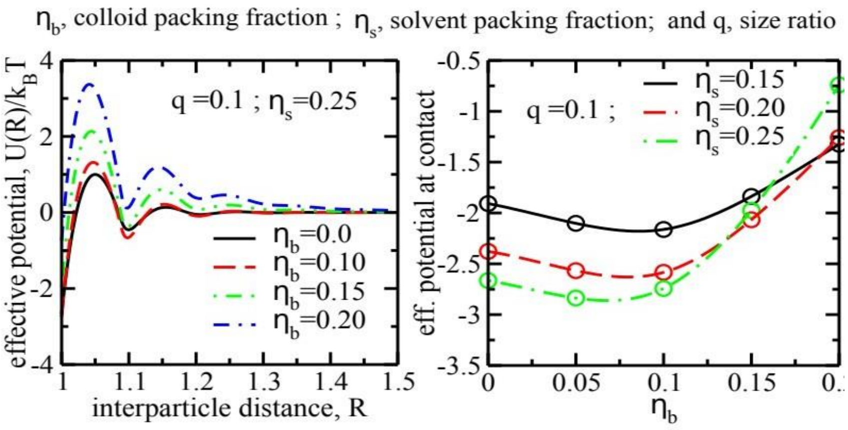

Figure 1: Effective interactions of a colloidal system.

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CO-P25

Synthesis of monodispersed Polyethylene nanoparticles by microemulsion

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359 million tonnes (Mt) of plastic is generated every year out of which 14.5 Mt has entered the ocean [1]. Around 30% of this plastic waste consists of Polyethylene (PE). This plastic waste in oceans commonly called as plastic marine debris (PMD) is exposed to physical, chemical and biological stresses which leads to fragmentation, forming micro and nanoplastic particles [2]. These particles are ingested by marine biota causing harmful effects whose repercussions in food chain are still unknown [3]. In our study, we try to synthesize Polyethylene nanoparticles (PENPs) using a novel o/w microemulsion (ME) system and hence using them to study their properties and characteristics. The spontaneous creation of nanometric domains in microemulsions greatly enhances their potential as nanotemplates for the synthesis of stable nanoparticles, owing to their cost-effectiveness and ease of preparation [4]. A suitable ME system was chosen and PENPs were synthesized by dissolving PE in an appropriate solvent and later stabilizing it with a water and surfactant mixture. Further, we aim to develop monodispered PENPs by varying the oil to water ratio, surfactant to water ratio, operating and synthesis conditions.

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Monitoring the MOF synthesis and quality using sessile drop drying phenomena.

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We demonstrate a new and simple technique to monitor MOF synthesis progress using the sessile drop drying phenomenon. UiO-66 MOF offers a wide range of applications with tunable chemical functionality and diverse structural topology [1]. The MOF (UiO-66) synthesis process involves different sizes and physicochemical natures of particles in every synthesis step. Using this nature of MOF synthesis with self-assembled patterning of a drying droplet, we were able to devise a potential tool for reaction analysis and purification. Physical parameters like temperature, impurities, the elastic modulus of the substrate, and deposited materials significantly affect the evaporation dynamics and particle transportation, thus affecting the final patterning [2]. We found that an equal weight percentage of purified-pore-activated and pore-inactivated MOF gives different deposition patterns when the well-dispersed aqueous droplet of these materials dries over various substrates. Our retro inspection study shows that the unreacted zirconium salt trapped in inactivated UiO-66 MOF causes the crack formation in the deposited film [3]. The presence of tetravalent ionic Zr-salt in the case of inactivated MOF dispersion partially neutralized the colloidal surface charge. It reduced interparticle electrostatic repulsion, positively attributed to the micro flocculation, and resulted in efficient close-packing of the MOF particle while drying. With efficient close packing of the MOF particle, the particle volume fraction (ϕ) increases, increasing shrinkage stress (σ_S). The stress (σ_S) gets relaxed by crack formation on the drying colloidal film [4],[5]. We investigated the mechanism of crack suppression with the help of Marangoni flow by increasing the substrate temperature during drying. We also observed different types of cracks by varying the substrate elastic modulus (glass and PDMS).

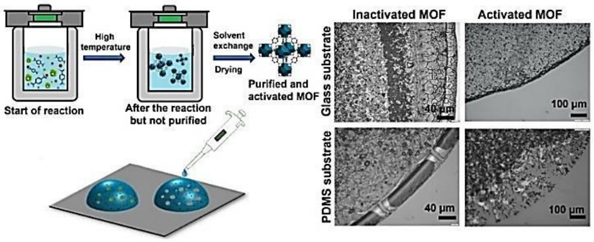

Fig 1: Schematic of our newly developed reaction progress monitoring tool using droplet drying.

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CO-P27

Phase Separation in Binary Strongly Coupled Plasma

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Plasma is a collection of charged particles (electrons and ions) that behave collectively due to electromagnetic interaction. The collective dynamics include plasma instabilities, waves, etc. The average coulomb potential energy is comparable to the average thermal energy in a typical plasma. However, when the Coulomb interaction energy dominates over the thermal energy, the particles tend to arrange themselves in more ordered structures resulting in the phase transition and intermediate states. They are classified as the family of strongly coupled plasmas (SCPs). This unique feature of such plasmas aligns them with soft matter physics like colloids and granular media.

This poster presents the phase separation phenomena using molecular dynamic (MD) simulation [1] in a binary strongly coupled plasma (BSCP) where particles interact through a derivative form of Coulomb potential. MD provides insights from particle to system size dynamics, thus making it appropriate to model such plasmas.

We observed that as the coupling strength of the system is increased, there is a notable reduction in the domain growth rate. In other words, as this coupling strength becomes more pronounced, the expansion of distinct domains within the system becomes increasingly restrained. This phenomenon indicates that stronger inter-component interactions relative to thermal fluctuations lead to a dampening effect on the growth of these distinct domains, resulting in a more constrained and less rapid evolution of the system's structural patterns over time.

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CO-P29

DYNAMICS OF PARTICLES IN LINE PLUMES

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We present a study of particle dynamics in line plumes with a uniform heat flux **Q** at the source to observe dust free regions with these plumes. We obtain a novel dimensionless form of the Maxey-Riley equation of particle motion by including thermophoretic force and normalizing the equation with the near wall length scales of Townsend, 1958. The particle motion is shown to be dependent on the modified Stokes number ($\mathbf{St_m=0.5(2+\varepsilon)C_BSt}$), the flux Rayleigh number ($\mathbf{Ra_f= (g\beta y^3Q)/(\nu\alpha K_f)}$), the flux-thermophoretic number ($\mathbf{Th_f=(2C_BC_TPrQ)/(T_pK_f)}$), the Prandtl number (**Pr**) and the gravitation number ($\mathbf{Gn=((1\text{-}\varepsilon)C_BSt)/Fr^2}$). The dimensionless plume velocity fields are obtained from the similarity solutions of Gebhart, using the same near wall length scales. We then solve the dimensionless Maxey-Riley equation numerically, subjected to this plume velocity field to obtain the flow streamlines and the trajectory of the particles. Dust free regions are observed at the center line of the plumes at larger $\mathbf{Th_m}$.

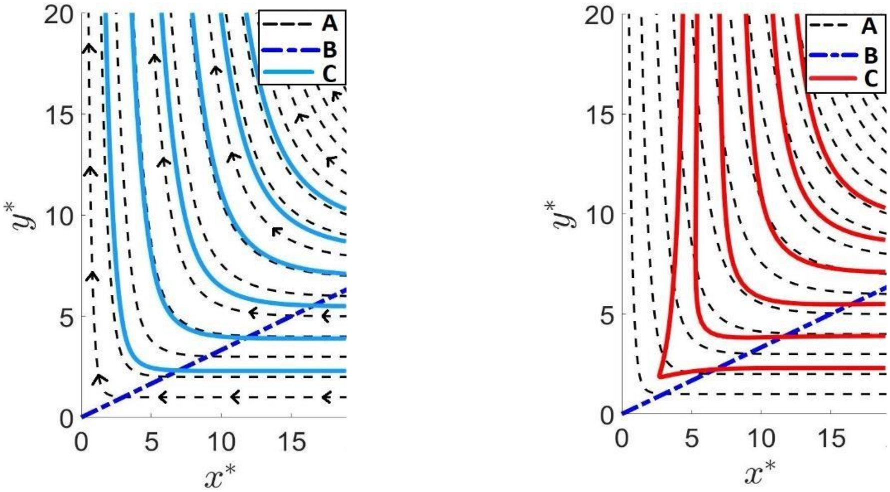

Figure 1: The left figure shows flow streamlines and particle paths at Pr=0.7; $Gr_g=10$; $St_m=10^{-5}$; Gn=0; $Th_m=0$. The right figure shows flow streamlines and particle paths at Pr=0.7; $St_m=10^{-5}$; Gn=0; $Th_m=0.3$; A = flow streamlines, B = Boundary layer edge, C = Particle trajectories.

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CO-P30

Tailoring the dimensions of silver nanowires (Ag NW) by modifying the polyol synthesis and the fabrication of Ag NW-based transparent conducting films

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One-Dimensional (1D) silver nanowires (Ag NWs) are widely used in the manufacture of flexible electronics.[1] This work describes an experimental investigation on tailoring the dimensions of Ag NWs by modifying the polyol synthesis. The polyol method is considered one of the most efficient synthesis routes for Ag NWs. This method uses ethylene glycol (EG) both as the solvent and a weak reducing agent for Ag^+ ions (typically from silver nitrate). A polymer, polyvinylpyrrolidone (PVP), acts as a capping agent to direct the 1D - growth of the nanostructures while metal halides, such as $FeCl_3$ act as growth promoters.[2] The reactions for the formation of NWs happen at elevated temperatures between 100-170 ° C.[3] The average diameter and length of NWs are tailored over a wide range, 35–150 nm and 12–130 μm respectively, by controlling the various synthesis parameters which include reaction time, temperature, molecular weight (MW) of PVP, binary mixture of PVP of different MW, and the concentration of NaBr. The effect of different metal halides (Cr, Cd, Cu, and Mn) as the growth promoters is also studied. Based on the experimental observations and hypotheses a growth mechanism is suggested for Ag NW formation in the solution phase. The synthesized Ag NWs are dispersed in isopropanol alcohol. This Ag NW dispersion is spin coated on the glass substrates to fabricate a transparent conducting film (TCFs). The optical and electrical properties are estimated to show its application as a TCF.

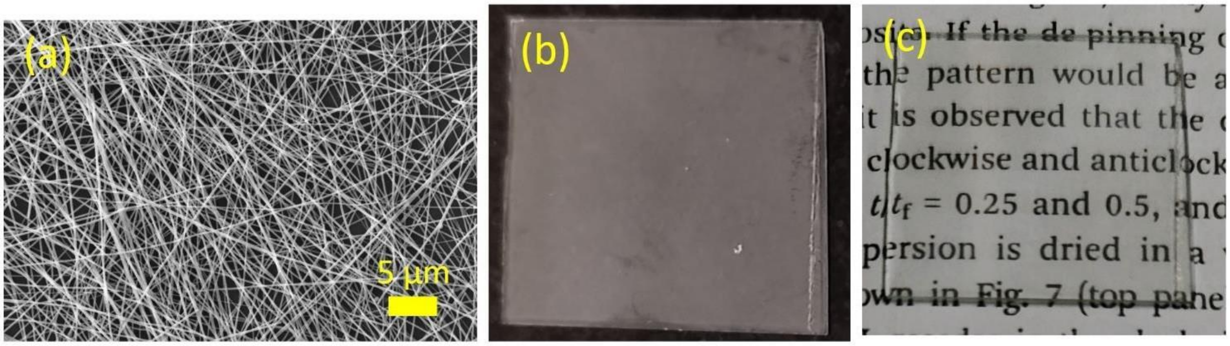

Figure 1: (a) Polyol synthesized Ag NW. (b) Transparent conducting film based on Ag NW made via spin coating, and (c) The thin film exhibits the transparency.

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All-natural Plant-derived Superhydrophobic Wax Coatings

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Plant-based waxes present a nature-inspired and environmentally friendly alternative to traditional synthetic hydrophobic coatings. Hydrophobic coatings, which repel water, are highly sought after for their ability to resist corrosion, self-cleaning properties, and effective oil-water separation, among other benefits[1].

In this work, the hydrophobic properties of organic waxes derived from lotus (Nelumbo nucifera) leaves, bauhinia leaves, and purple periwinkle (Vinca) flower petals will be presented. These substances exhibit natural hydrophobicity due to the presence of intricate nano/microstructures of cuticular wax on their surfaces[2]. Drop casting them onto glass substrates to form coatings allowed for a comparison of extraction time, hydrophobic characteristics, thickness, and wax recrystallization rates. The coatings were observed to achieve effective water repellency on hydrophilic substrates. Optimal concentrations and thicknesses were determined and the results were substantiated by the degree of wax recrystallization.

Noteworthy results include the outstanding 150° static contact angle values achieved by 15 mg lotus wax dissolved in chloroform solvent, in contrast to bauhinia and periwinkle coatings which exhibited ~110° contact angles only. This work opens the door to crafting sustainable hydrophobic coatings from natural sources that have zero potential for secondary contamination.

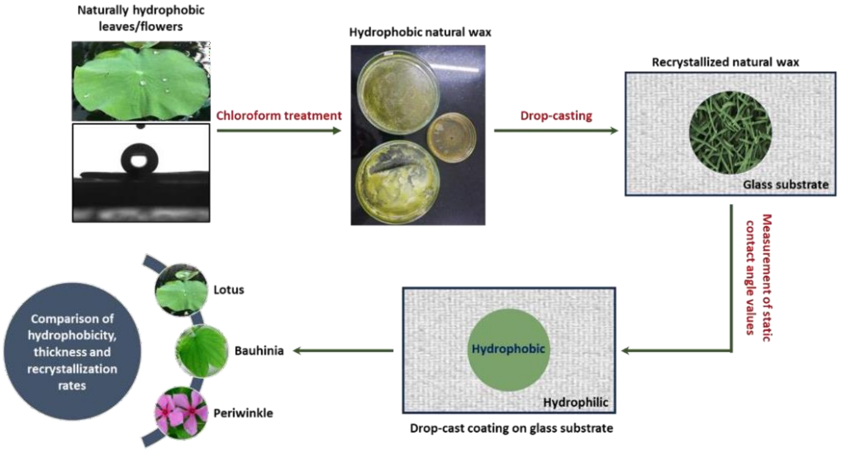

Figure 1: *Schematic of drop-casting natural wax to create hydrophobic coatings*

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Indian Society of Rheology

CO-P34

Plasmonically controlled patterning of metallic nanoparticles at liquid-liquid interface

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The fluid-fluid interface is emerging as a promising soft substrate for realizing micro/nanoparticle assembly. Though the platform is utilized as reconfigurable optical modulators [1], tunable plasmonic mirrors [2], and SERS substrate [3], the on-demand patterning of nanoparticles remains unaddressed. The light-controlled flow based patterning techniques are particularly interesting as it ensures on-demand, contactless patterning in a programmable manner [4], [5]. Herein we develop a novel light-controlled liquid-liquid interface mediated method for the on-demand patterning of metallic nanoparticles. The system comprises heptane (top layer), water (bottom layer), and gold nanoparticles (Au NPs) layer at their interface. The principle relies on the controlled displacement of nanoparticles assembled at the liquid-liquid interface based on plasmonically-controlled thermocapillary flow (Figure 1a). By merely changing the optical landscape, we have achieved different patterns such as single spot (Figure 1b), two spots, and three spots.

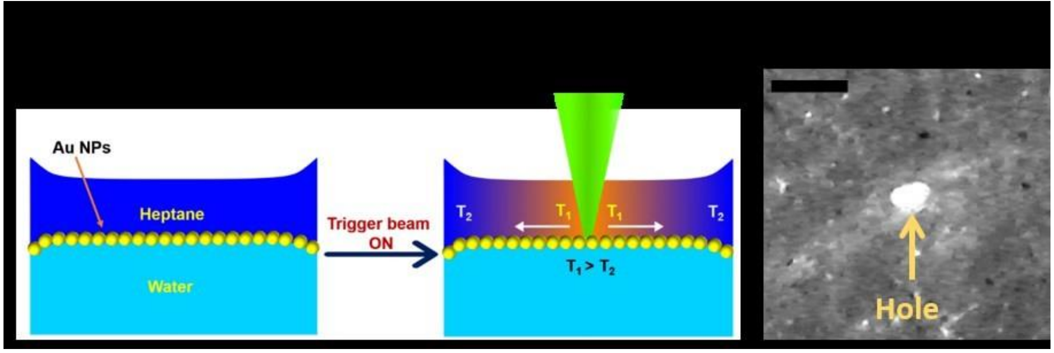

Figure 1: a) Schematic showing the principle of optically controlled thermocapillary flow. b) Optical image of gold nanoparticles (Au NPs) layer captured in top view mode under single spot illumination. Scale bar corresponds to 0.5 mm.

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Indian Society of Rheology

CO-P35

Pattern formation in microgel laden sessile droplets: Effect of substrate temperature

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Drying of a particle-laden droplet on a substrate leaves behind a particulate deposit whose morphology depends on a multitude of factors, including inter-particle interaction, substrate wettability, substrate orientation, ambient conditions, particle-solvent interaction, and substrate temperature. During the evaporation of a droplet, capillary force, Marangoni force, and droplet dynamics affect the final deposit pattern. Generally, capillary force exerts a predominant influence, giving rise to the commonly observed coffee-ring deposits. However, the Marangoni force becomes significant when temperature or particle number density gradients exist between the droplet's apex and contact line, leading to alterations in the deposit configuration. Zhong and Duan [1] reported the transformation of the particulate deposits from a disk-like pattern to a dual-ring pattern by varying the substrate temperature. Another study by Lama et al. [2] revealed that the central depletion zone of a particulate deposit can be adjusted by manipulating particle concentration and substrate temperature.

In this investigation, we will elucidate the correlation between deposit patterns resulting from drying microgel-laden aqueous droplets and the substrate temperature. Given that PNIPAM microgels exhibit a Volume Phase Transition Temperature (VPTT) at 32°C and tend to adsorb at the air/water interface during droplet evaporation [3], varying the substrate temperature over a range encompassing both below and above ambient conditions will not only influence deposit patterns but also impact droplet dynamics. A comprehensive analysis of how the morphology of the deposit obtained by drying microgel-laden aqueous droplets can be modulated by meticulously adjusting the substrate temperature and particle concentration will be presented in detail.

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CO-P36

Coffee stain morphologies obtained by drying suspension droplets of gold nanorods of different aspect ratios

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The evaporation of colloidal suspension droplet results in the deposition of the solute phase in coffee stain patterns. The dried deposits are interesting to study from the viewpoint of applications in biomedicine, nanotechnology, printing, coating, etc. We have synthesized aqueous colloidal suspensions of surfactant (CTAB) stabilized gold nanorods using a seed mediated growth method. The obtained gold nanorod aspect ratio has been tailored by varying the silver nitrate ($AgNO_3$) concentration for small aspect ratios and surfactant ratio (BDAC/CTAB) for high aspect ratios. The formation of gold nanorod of different aspect ratios was confirmed using UV-Visible spectroscopy measurement and the nanorod size and morphology were studied using scanning electron microscopy (SEM). We are studying the evaporation kinematics at room temperature using a contact angle meter and the final coffee stain patterns that are left behind after solvent evaporation using SEM. We find that the evaporation of a sessile suspension droplet of gold colloidal nanorods results in coffee stain with formation of various distinct regions. Our preliminary results show an enhancement in ordering of the self-assembled structures with increasing nanorod aspect ratio. Also, there are distinct depinning behaviour is noted for suspensions of different aspect ratio gold nanorods.

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Indian Society of Rheology

CO-P37

Non-linear fluctuating hydrodynamics of a colloid near a plane surface

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We study trapped colloidal particles undergoing forced oscillations near fluid boundaries that show harmonic generation. This harmonic generation is a product of non-linear near-field interactions happening very near the fluid boundary, which causes the mobility of the colloid to change significantly from that of the fluid bulk. We use theoretical models and simulation to arrive at a best-fit explanation for the harmonic generation near fluid-solid and fluid-air interface boundaries.

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CO-P38

Slow dynamics of a soft glassy colloidal suspension in the presence of probe particles

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Supercooled liquids, in general, show increase in their viscosities and structural relaxation times when quenched rapidly towards their glass transition temperatures. In this work, the dynamics of aging Laponite suspensions (a model glass former) with dispersed polystyrene (PS) beads used as probe particles, is studied in dynamic light scattering (DLS) experiments. In an earlier work, our group had demonstrated a one-to-one mapping between the aging time of a colloidal Laponite suspension and the inverse of the temperature of a molecular glass. Intensity autocorrelation functions measured in DLS experiments show the existence of two-step relaxation processes in these suspensions. The PS beads, being less mobile and larger in size than the Laponite particles, diffuse very slowly and act as nearly pinned particles in the Laponite suspension, with the diffusion time of PS beads being significantly higher (nearly two orders of magnitude) than Laponite particles. The fragility parameter D and Vogel time tα□, which quantify the approach of the aging Laponite suspension towards eventual kinetic arrest, are calculated from the evolution of the structural relaxation time for different concentrations and sizes of probe PS beads. Initial experiments suggest a good match of our experimental data with existing theoretical predictions.

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CO-P39

Quantitative Characterization of Deposit Patterns Formed from Dried Dispersion Drops

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Abstract:

Coffee rings[1] or coffee stains are patterns left behind by the solvent evaporating from particle-laden sessile drops. The particles in the dispersed medium are carried away to the edge by the capillary force that arises as the drop evaporates. This phenomenon affects the overall working of industrially relevant processes such as inkjet printing[2], disease diagnosis[3], etc., and various attempts have been made to control it depending on the application. Although innovative work has been done in this field, the characterization of the spatial distribution of patterns is still primarily qualitative. Therefore, in this work, we propose a method to quantify patterns formed from dried drops using a radial distribution parameter m_r and an azimuthal distribution parameter m_θ. While m_r captures the extent to which the particles are at the edge and away from the center, m_θ provides information on how clustered the particles are at a given radial location. These parameters combined can be used to numerically represent the overall distribution of particles in deposit patterns.

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CO-P40

Reversibly
Aggregating Binary Colloidal System

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We report the structural study of reversibly aggregating binary spherical colloidal particles using Brownian Cluster Dynamics (BCD). It is shown that the local free space available to particles is an important control parameter for aggregation. Further, as presence of one type of species influences the free space available to another, there is a high correlation between the aggregation of individual species even in the specific case of A-A and B-B bonding, without A-B interaction, where A and B denote the two different types of particles which are structurally identical. Moreover, the phase diagram of the binary system shows a remarkable difference from the monomeric system.

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CO-P42

Enhancement in the transport properties of a tilted rough ratchet

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The phenomenon of Brownian motion in a periodic washboard potential has been of long-standing interest to scientists for decades. In the literature, most studies have focused on diffusion in the presence of a smooth potential. However, in most cases, these particles come across surfaces that are rugged or rough on a microscopic scale. Moreover, due to different factors, there are perturbations in the energy landscape of various Physical, Chemical, and Biological processes [1]. The transport of particles in the presence of such rough energy landscapes is of great importance.

In this work, we delve into the transport properties of a Brownian particle in a rough washboard potential via Brownian dynamics simulations. The diffusion coefficient, particle current, and Peclet number are examined in this work as functions of various system parameters. Prima facie, it would appear that roughness in the potential would hinder diffusion [2] and reduce the particle current. But in some cases, the roughness improves the particle current [3]. However, our results show that at low temperatures and in a particular range of spatial frequencies of rough potential, the amplitude of the roughness in the potential promotes the diffusion [4] and, in a particular domain of system parameters, roughness also enhances the particle current.

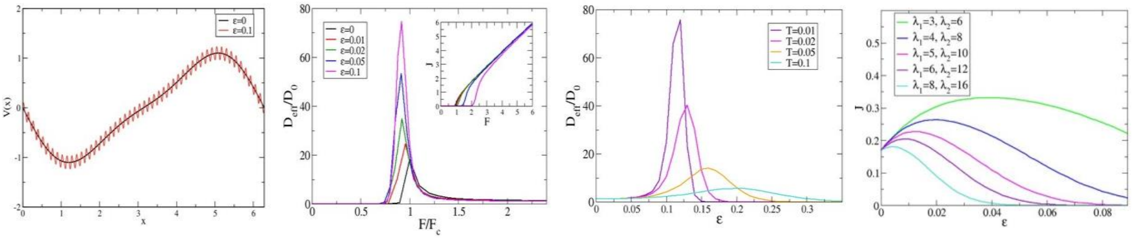

Figure 1 : a)The potential V(x) in the absence and presence of roughness. b) D_{eff}/D_0 as a function of tilting force F at temperature T=0.01 Inset : J versus F at T=0.01 c) D_{eff}/D_0 as a function of the amplitude of roughness □ when F = 2.5 . d) J versus □ when F=0.01 and T=0.01.

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CO-P44

Sphere motion in a viscous, stratified fluid

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The study of the flow-field around a sphere settling in a viscous density-stratified ambient is an interesting one due to the complicated flow physics arising from the interplay of viscous, buoyancy and inertia forces. It is also an important one since, among other things, the "Biogenic mixing hypothesis" [1, 2] proposes the drift volume associated with vertically migrating zooplankton as being a major contributor to oceanic mixing. In this study, we present salient features of the disturbance flow field due to a sphere moving vertically in a viscous stably stratified ambient [3]. When viscous and buoyancy forces are in balance, we show that the flow field is highly non-trivial, characterized by the presence of primary, secondary and tertiary screening lengths. We also trace the fluid pathlines in an attempt to quantify the drift volume over a wide range of viscous Richardson numbers. The total drift volume turns out to be anomalously small, contrary to naive scaling estimates. We then examine the flow-field for the case where inertia and buoyancy forces are in balance at large distances, and quantify the drift volume for this oceanically more relevant scenario.

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Synthesis and Characterization of 2D Colloidal Sheets

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Colloidal particle assemblies provide a useful model for understanding molecular systems. Moreover, these assemblies hold promising applications in technology, spanning electronics, biomedicine, and optics. Previous studies have demonstrated assembly of colloidal particles in the form of 1D colloidal chains, that represent models for polymer chains [1-3]. The size of the colloid is advantageous, being small enough to exhibit Brownian motion yet sufficiently large for microscopic observation. Similarly, colloidal sheets can serve as analogues of molecular 2D materials.

To this end, we have developed a novel method to synthesize 2D colloidal sheets. This involves assembling polyethyleneimine (PEI)-coated colloidal particles, such as silica or polystyrene, into a 2D plane and then crosslinking PEI. A sessile droplet of PEI-coated colloidal suspension was evaporated on an oil-coated surface. The air-water-oil contact line is not pinned but continually moves inward as the droplet evaporates. This suppresses the coffee-ring effect. The internal flow driven by the motion of contact line pushes particles towards the water-air interface. The nature of particle assembly at the water-air interface depends on initial particle number density. At sufficiently high particle number densities (particle volume fraction 1.75×10^{-6}), colloidal particles assemble at the interface to form 2D crystalline domains. As evaporation progresses, these crystalline domains are pushed together to form a close packed "colloidal skin". At the end of drying, a colloidal sheet with polycrystalline domains is formed. As initial particle number density decreases, fewer crystalline domains are formed and crystallinity of the sheet decreases. At lower initial particle number densities (particle volume fraction 5.67×10^{-9}), no crystalline domains are formed. Instead, an amorphous colloidal sheet is formed at the interface at the end of the evaporation. Thus, the crystalline order in colloidal sheet can be tuned by changing initial particle number density.

By particle tracking of fluorescent markers present on the sheet, we observed that the fluctuations in the distances between the markers increased when the cross-linker-to-PEI ratio is decreased. This demonstrates that the effective in-plane flexibility can be tuned by amount of cross-linker. Additionally, by selective dissolution of polystyrene particles in polystyrene-silica composite sheets, we synthesized colloidal sheets with holes as analogues of porous molecular membranes.

We intend to explore the influence of local features such as bead size, rigidity of inter-bead bonding, and the presence of holes on the overall mechanical properties of the sheets.

Keywords: 2D Materials, Colloidal Sheets, Polymer Coated Colloids

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Micromechanics of particulate soft matter: the governing role of inter-particle interactions

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The advancement of humanity has been closely tied to material revolutions throughout history. Eras were named after the materials that defined them, such as the Stone, Copper, Bronze, and Iron ages. Today, we are in an era of "Soft Materials," including particulate suspensions, colloids, polymers, surfactants, liquid crystals, and living matter. These materials are found in everyday objects, from consumer products like inks, paints, soaps, and food items to sophisticated technology like displays, batteries, and pharmaceutics. This talk focuses on particulate soft matter, viz., suspensions or colloids. Controlling the flow of suspensions is a crucial piece of an unresolved puzzle in many applications, e.g., biofuel production, solar cells, electronics cooling, and fiber-reinforced thermoplastics. Unraveling the underlying fundamental mechanometric principles that determine such materials' behavior and exploring ways to tune them is thus crucial to increase the efficiency and throughput of processes involving such particulate suspensions. To this end, we developed an experimentally validated and physics-based computational approach to study the flow of dense suspensions near jamming limits and quantitatively determined the role of inter-particle interactions on the rheology, the jamming fraction, and the microstructure of dense suspensions [1]. These investigations elucidate the heterogeneous and hierarchical nature of structural and dynamic complexity in suspensions across scales, from microscopic to macroscopic.

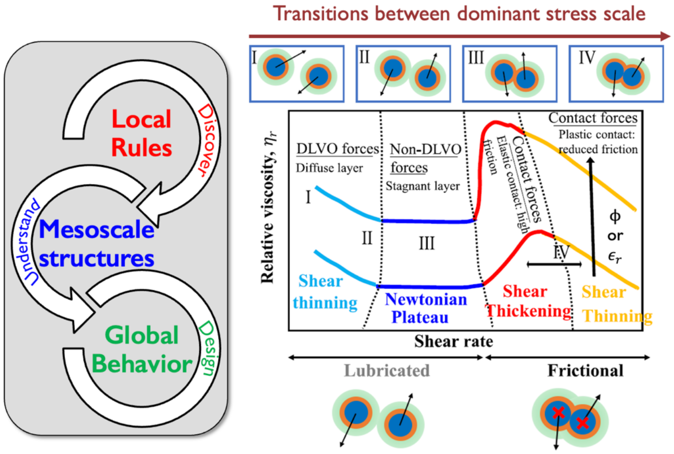

Figure 1: Effect of various interparticle interaction in determining disparate rate dependent regimes in the flow curves of dense suspensions and the corresponding transitions, which happen due to transitions in the dominant force in the system [2].

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Unveiling the Self-Pinning Driven Jamming Behavior of Colloids during Droplet Drying

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The drying of colloidal droplets leads to the formation of intricate patterns, a commonly observed phenomenon in our everyday lives and advantageous in various research and industrial domains including inkjet printing, spray coating among others. Despite it seemingly straightforward nature, the drying of the colloidal droplets is profoundly influenced by the properties of the colloidal fluids and intricate interactions within the system. The jamming of colloidal particles within a dried droplet depends on several factors, with the wetting of the substrate and motion of the three-phase contact line playing a crucial role. When a droplet dries on a substrate, the suspended colloidal particles are deposited along the droplet's edge, causing the contact line to become pinned. This pinning of contact line results in non-uniform evaporation of the solvent from the drop-air interface with a consequential outward transport of the colloidal particles and an accompanying increase in the velocity of the colloidal particles.

A research question arises: Does the velocity of colloidal particles increases during the drying of the colloidal droplet on a superhydrophobic (SH) surface as well as for the air suspended colloidal droplets? To address this question, a study was conducted utilizing electron microscopy and Small-Angle X-ray Scattering (SAXS) to examine the jamming behavior of the colloids in droplets dried on SH surface as well as for the air suspended droplets obtained via spray drying.

The resulting supraparticles obtained from the evaporation of the droplets on the SH surface as well as via spray drying, exhibit a localized arrangement on the outer surface, while the arrangement becomes random in the inner region. During the initial stages, as the solvent evaporates from the drop-air interface, the droplet interface recedes and colloids diffuse toward the interface, leading to the formation of an ordered shell. This shell formed at the interface acts as self-pinned contact line, preventing any further recession of the droplet-air interface. However, the formation of the menisci between the colloids serves as nanomembranes and the solvent evaporation occurs through nanopores. This evaporation process is rapid, resulting in an increased velocity of the colloids, transporting them outward and leading to a random arrangement of the colloidal particles within the inner region.

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EC-O4

Morphogenesis of active fluid surfaces: a mechano-chemical model

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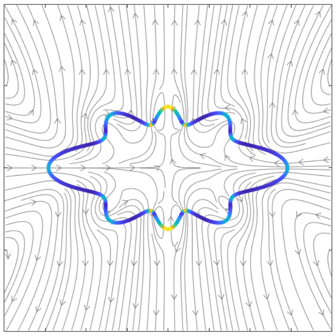
Eukaryotic cells exhibit remarkable chemical and morphological patterns on their surface which are responsible for many of their biological processes such as cell division. It is becoming increasingly evident that physical mechanisms including intracellular mechano-chemical forces and fluid flow are responsible for this self-organized behaviour. By modelling the cell membrane as an active fluid surface[1,2], we study the coupled dynamics between the transport of force-inducing molecular species and the surface deformation. A unified numerical framework based on the Boundary Element Method is developed to efficiently compute the flow-fields and the non-linear dynamics of the surface.



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EC-O5

Sequence-specific folding of active macromolecules

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Many of the important physical properties of biological polymers such as actin filaments and microtubules are due to their out-of-equilibrium behavior induced by ATP (Adenosine triphosphate) or GTP (Guanosine triphosphate) [1]. Whereas, synthetic polymers capitalize on available energy sources in the environment and generally contain components that are driven far-from-equilibrium by exploiting local chemical, electrical or thermal gradients [1]. On the theoretical front, active polymers are a minimal model of such macromolecular materials where the competition between thermodynamic and active forces can be systematically studied in a system that also undergoes conformational transformations.

In our study, we perform numerical simulations of an active polymeric chain of multiple self-avoiding units. We find that a judicious inclusion of active forces perpendicular to the chain backbone according to specific patterns can generate designable and reconfigurable two-dimensional folded structures [2]. We observe the existence of an ensemble of highly mobile compact structures capable of moving from one conformation to another. Furthermore, extending our investigation to partially active polymers without particular orientational constraint, we discover that distribution of the active units in distinct sequences along the backbone is still able to induce a significant collapse into folded globular structures. A detailed analysis reveals that this activity dependent structural change is in fact driven by a negative active pressure between the monomers. Overall, our study demonstrates a direct correspondence between the sequence and orientation of the active forces and the structure of folded conformations in macromolecular active systems.

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Spatio-temporal dynamics of nutrient exchanges in microbial active matter

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Microorganisms inhabit highly fluctuating environments and survive in a low-nutrient resource bath. It is now recognized that symbiotic relationships between microbes play a vital role in their survival. The existence of such interaction raises general questions about the spatio-temporal dynamics of nutrient exchanges. Here we experimentally and theoretically examine a model system of this problem – *bacteria*, an obligate microbe capable of chemotactic response towards the green *algae*. Even in their simplest arrangement in a localized domain, we find a complex dynamics involving nutrient exchanges, enhanced algal diffusivity due to the bacteria, and a stochastic version of "flux expulsion".

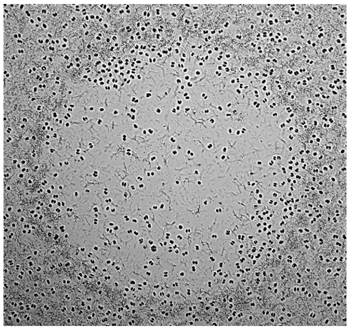

Figure 1: Flux expulsion of algal cells (dark spots: ~7 μm) due to enhanced diffusion by bacteria (tiny speckles ~1.5 μm).

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Role of Contact Inhibition of Locomotion in collective behavior and de-mixing of cell types

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Contact inhibition of locomotion (CIL) is a fundamental process in cell-cell interactions and plays a crucial role in biological phenomena such as wound healing, cancer metastasis, tissue development etc. Similar to Vicsek model [1], we simulate the effect of CIL by modeling the cells as self-propelled disks which obey overdamped Langevin dynamics in crowded environment. We update the positions and orientations of cells through computer simulations using the mathematical model we designed.

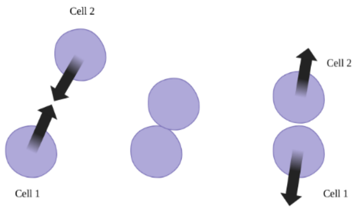

Figure 1: Illustration of contact inhibition of locomotion between two cells.

Many interesting results regarding dynamics of cell colonies such as cell dispersal, collective migration [2], phase separation from gel-like structures to polar fluids and de-mixing of healthy and cancer cells are studied through rigorous computer simulations and analytical techniques, which we intend to present at the conference.

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EC-P2

Indian Society of Rheology

Nucleation in the presence of static/dynamic impurities with varying interaction strength in an Ising lattice-gas model of solute precipitation

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Nucleation is often observed in nature and the presence of impurities in every real and experimental system is unavoidable. Impurities play a major role in the nucleation process. It could speed-up or slow-down the nucleation rate depending on the nature of interaction. We have studied the behavior of the droplet free energy and nucleation rate in two dimensional Ising lattice-gas with varying interaction strength in the presence of randomly positioned static/dynamic impurities. For the static case, the barrier height decreases with increasing impurity density enhancing the nucleation rate when impurities interact neutrally with both solute and solvent. The rates obtained using the simulation (forward flux sampling method) fit a Becker-Doring expression for different impurity densities [1]. In the case of dynamic impurities, at low temperatures ($1/k_B\beta$) we observe preferential occupancy of the impurities at the boundary positions of the nucleus enhancing the nucleation rate by lowering of the effective interfacial free energy [see snapshot in Figure1(b)]. Further, we simulate the system for different interaction coupling strengths of the impurity with solute (J_+) and solvent (J_-) particles [see Figure 1(a)]. Depending on the positional occupancy of the impurities, we find three regions in the parameter space. These are, regions where impurities prefer to inhabit the solute phase, the solvent phase, and the boundaries. We also observe a saturation in barrier height with decreasing symmetric interaction strengths ($J_+=J_-=j$) for dynamic impurities which corresponds to the phase where impurities are completely excluded from the nucleus.

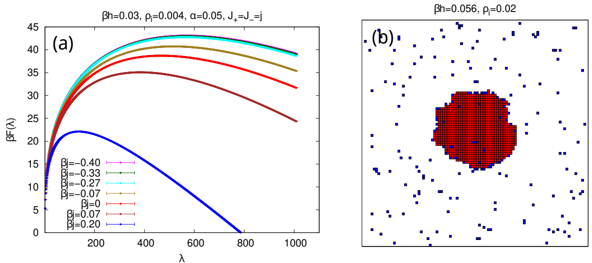

Figure 1 (a) Nucleation free energy $\beta F(\lambda)$ as a function of cluster size λ in Ising lattice-gas model with external field $\beta h=0.03$ for different symmetric interaction strength βj in the presence of dynamic impurities of concentration $\rho_i=0.004$. (b) Snapshot of a typical configuration showing the cluster (red) with impurities (blue) occupying boundary positions for $j=0$.

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EC-P3

A Computational Study on the Smooth-Wall, Radial Gravity Phenomenon in Granular Flow Through a Wedge-Shaped Hopper

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Hoppers with inclined walls are used in industry, where materials flow by gravity and exit through a bottom outlet. The simplest form of this flow can be described as a wedge-shaped, quasi-two-dimensional geometry with smooth walls, influenced by radial gravitational forces. Theoretical analysis of this flow has been conducted using the Mohr-Coulomb criterion in the classical work of Savage (1965) and using a critical state theory by Ravi Prakash and Rao (1988). To validate the existing theories, discrete element method simulations are performed on particles within a smooth-wall radial gravity wedge-shaped hopper, obtaining detailed stress and velocity fields. Our computational results match with the predictions of the existing theories, except in the region near the exit where both frictional and viscous effects are present. To further understand this behavior, we conducted a parametric study on wedge-shaped hoppers, varying parameters such as orifice size, wedge angle, friction coefficient, and stiffness. This study investigates the influence of frictional walls and vertical gravitational forces on the system's behavior, aiming for a comprehensive understanding. The transient outcomes are compared to the average behavior to deepen our understanding, and the results are presented. And also, empirical correlations quantify the relationships between stresses at the exit, considering frictional and viscous forces. In particular, the correlation between viscosity and shear rate at the exit is important, as it captures the effects of momentum and particle transfer during collisions, exhibiting a significant dependence on viscosity near the exit region. Additionally, it is demonstrated that viscosity and volume fraction exhibit power law correlations with the inertial number proposed by Jop et al. (2006) and that all the data collapse into a single curve, enhancing our understanding of granular material behavior for such flow prediction.

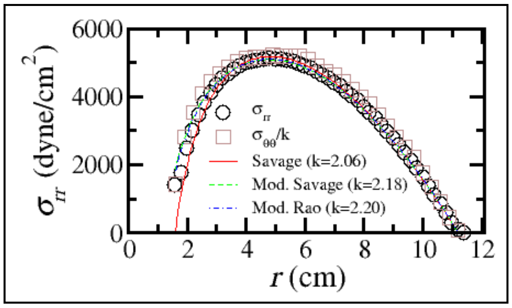

Figure 1: Stress in *r-direction* as a function of radial diatance.

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EC-P4

Effect of Coarse Particle Shape on Mixing and Segregation Dynamics: Insights from Experimental and Discrete Element Method Analyses

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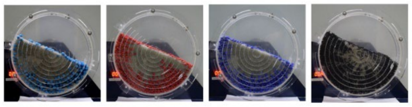
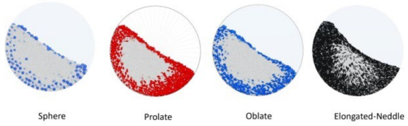
Solid-solid mixing is a fundamental process utilized across numerous industries, yet a comprehensive understanding of granular material behavior remains elusive[1]. This study employs the Discrete Element Method (DEM) to explore the progression of radial segregation and its relation with variations in particle shape. By generating four distinct types of binary mixtures, the investigation emphasizes the significant role of coarse particle shape in governing mixing and segregation dynamics within a rotating drum. The initial homogeneous blending of coarse and fine particles gives way to radial segregation, marked by the aggregation of fine particles at the drum's core, surrounded by coarser counterparts. Notably, the study unveils that spherical particles, whether act as coarse components in binary mixtures, tend to encourage segregation. Additionally, the study identifies that elongated needle-shaped particles exhibit relatively enhanced mixing behavior compared to spheres. This trend is consistent across both experimental and numerical simulations, displaying a successive reduction in the segregation index value: sphere, followed by oblate, then prolate, and finally elongated needle for the coarse particles. Figure 1 shows the post visualization snapshot configuration of the binary system, featuring four diverse shapes of coarse particles with fixed fine particles.



(a) Experimental



(b) Numerical (DEM)

Figure 1: Post-rotation visual comparison of particle distribution, displaying (a) experimental results and (b) DEM simulation outcomes.

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EC-P5

Drug Delivery from Ocular Implant: An In-silico Investigation

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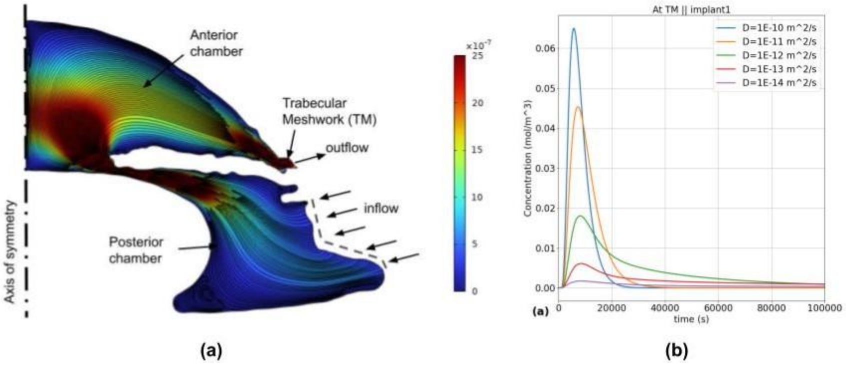
Drug-loaded implants (DLIs) have the potential to serve as a viable alternative to the conventional methods of administering ocular drugs, such as topical and oral delivery. The utilization of drug delivery systems, such as DLI, offers several notable benefits. These advantages include the ability to circumvent numerous biological barriers, a reduced risk of systemic toxicity, and the elimination of the requirement for patient adherence to delivery protocols. In order to facilitate widespread utilization, it is necessary to optimize the duration during which implants can effectively release drugs within therapeutic limits. With this goal, we decided to model and simulate the flow of aqueous humor (AH) and drug administration from several types of implants inside the anatomically realistic geometry of the human eye, see Figure 1(a) [1]. Specifically, we focused on the effects of effective diffusivity, implant's shape and size, and implant placement. Results suggest that effective diffusivity (D_{eff}) has the most dominant effect on drug release and time period over which drug remains in the therapeutic window. For example, drug delivery from an implant to Trabecular Meshwork, loaded with 10 μg of drug, remains within therapeutic limits only for a few hours in case of D_{eff} = 1E-10 m^2/s but nearly a month for D_{eff} = 1E-14 m^2/s, see Figure 1(b). The geometric properties of the implant and its placement affect the burst release and drug distribution in AH, respectively. Therefore, it is concluded that enhanced control over drug availability at a specific area can be facilitated by the target specific planning of many factors, including the implant's location, the effective diffusivity of the drug, and the shape and size of the implant.



(a) (b)

Figure 1: (a) Realistic geometry of anterior and posterior chamber of human eye filled with Aqueous Humor (AH) (b) Variation of drug concentration at Trabecular Meshwork with time for multiple effective diffusivity

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EC-P6

Indian Society of Rheology

Functionally graded shape reprogrammable liquid crystal elastomers films for artificial gripper applications

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Liquid crystal elastomers are a unique class of responsive materials showing large magnitude reversible shape deformations. The anisotropy and elasticity render these materials useful in many applications such as responsive coatings, smart textiles, sensors and actuators etc. In this work, we prepare a liquid crystal elastomer gripper using two step thiol- acrylate crosslinking. After the initial crosslinking, the oligomeric film is molded to a desired geometric shape and then cured under UV light for the final crosslinking. The degree of crosslinking changes through the length of the film. It was achieved by employing different UV intensities during the second step of crosslinking at selective locations and masking the rest of the film. As a possible application, we show the gripping action of the film. The gripper demonstrated here is seamless and not engineered by joining more than one responsive film.

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EF-O2

The effect of interfacial stresses on film drainage

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Thin liquid film (TLF) dynamics is considered to be the governing factor when it comes to the stability of multiphase materials, such as foams, emulsions and immiscible polymer blends. When two bubbles come into close proximity a TLF is usually formed between them, which gradually drains. The drainage process and, consequently, the stability of TLFs has been found to depend heavily on the surface stresses. However, the exact ways by which surface stresses due to Marangoni, surface viscosity and surface viscoelasticity act remain unclear. In this study we employ novel experimental protocols using the dynamic thin film balance technique [1] to study how exactly surface stresses affect the drainage. Three different surfaces were studied in a wide range of Capillary numbers, namely a low molecular weight non-ionic surfactant (Marangoni stresses) at three different concentrations, hexadecanol (surface viscous), and polymer multilayers (surface viscoelastic). Film visualization was done using microinterferometry. The use of model systems allows us to decouple the effects of disjoining pressure, surface stresses, capillarity and hydrodynamics [2]. We show that the drainage behaviour is markedly different among each film, depending both on the magnitude and the type of surface stresses. The different spatiotemporal evolution of the latter results in variations in the shape of the films. Previous, seemingly contradicting, results in literature are rationalized and the limitations of existing practices in droplet coalescence studies are discussed.

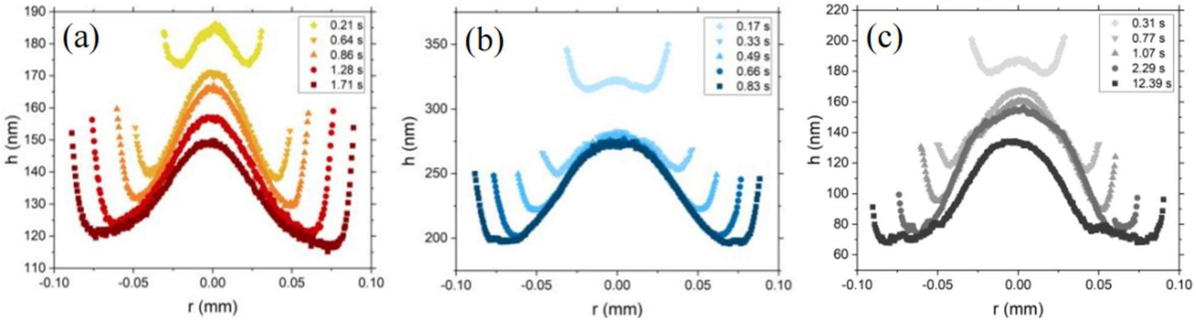

Figure 1: Thickness profiles of draining films stabilized by different surface stresses. (a) Marangoni stresses, (b) surface viscosity, and (c) surface viscoelasticity.

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Use of Drop Rest Technique to evaluate the stability of waxy crude oil

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The petroleum industry frequently produces crude oil in the form of solid-stabilized W/O emulsion. Along with the natural surfactants in crude oil, colloidal particles such as asphaltenes, resins, and wax adsorb at the oil-water interface and create a rigid interface. Specifically, to comprehend the destabilization of wax-stabilized W/O emulsion, in waxy crude oils, it is critical to investigate the resistance coalescence process. So far, studies on the coalescence phenomenon have been done in model oils through optical observations using a high-speed camera due to the opacity of the crude oil to visible light. Therefore, to understand the water droplet coalescence at the crude oil-water interface, the present study has been done through "the Drop Rest Setup", using a Near-Infrared Camera (NIR). This setup offers the advantage of performing systematic measurements of a single droplet-interface interaction and yields the drop rest time distribution in the presence and absence of different surfactants. The drop rest time is the amount of time a droplet pauses at the interface before coalescing with the mother phase below. A broad rest time distribution was observed in a study of 90 droplets conducted in the presence of surfactants. This is attributed to the stochasticity associated with the nonuniform thickness of the interface, which gets altered by the addition of surfactants. The statistical model presupposes that a "third phase" at the interface prevents the aqueous drops, resting at the interface, preventing the coalescence of the aqueous droplet with the brine below. It is assumed that the interface is covered with a wax layer that is made up of interlinked wax particles. In the absence of surfactants, the adhesion between the adjacent wax crystals is sufficiently strong to prevent drop coalescence, except at very high temperatures. Based on these concepts, an analytical model for the distribution of rest times is suggested. The model explains the results of our experimental work.

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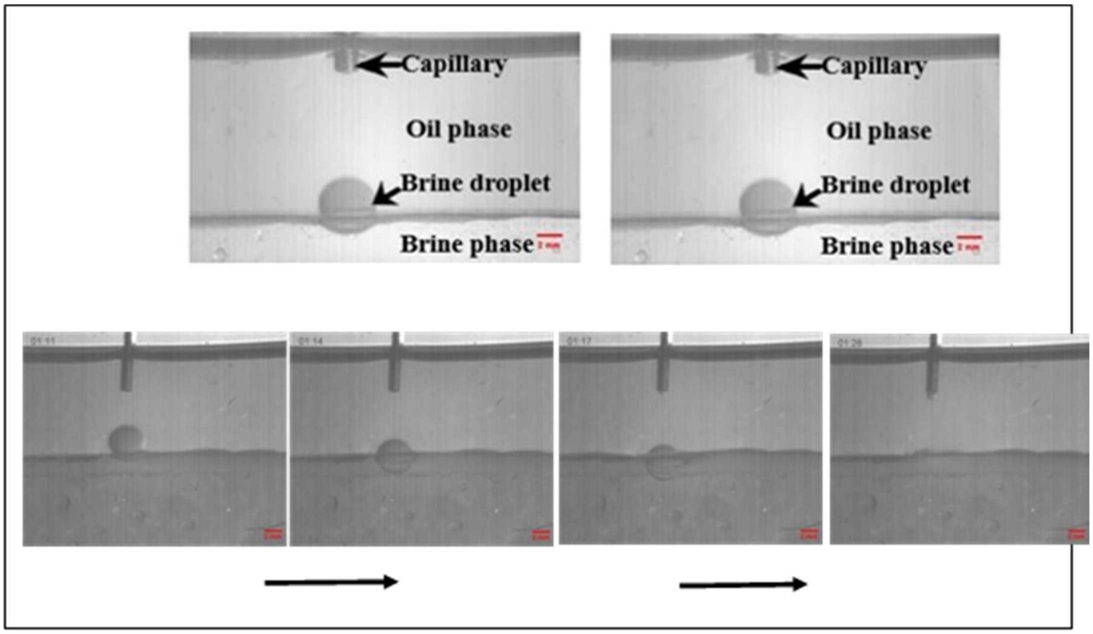

Figure 1: Drop Rest (a) in the absence of surfactant (b) in the presence of surfactant

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EF-P7

Light-induced destabilization of oil-in-water emulsions using light-active Bolaform surfactants.

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External stimuli-induced destabilization of oil-in-water emulsions is of both fundamental and technological importance. In this work, we have synthesized light-active Bolaform-surfactants (LABSs) and demonstrate their use in preparation of decane-in-water emulsions over a range of surfactant and salt concentrations. Under ultraviolet (UV) illumination, LABSs undergo trans to cis isomerization affecting their interfacial activity. Therefore, when stable emulsions stabilized by LABSs are exposed to UV light, they undergo partial destabilization. To induce interfacial flow, a small amount of volatile solvent (methanol, ethanol, tetrahydrofuran, etc.) is added at the emulsification stage and in this case complete phase separation is observed. This study demonstrates a facile route to induce destabilization of surfactant-stabilized emulsions using benign solvents and minimal use of energy (UV light).

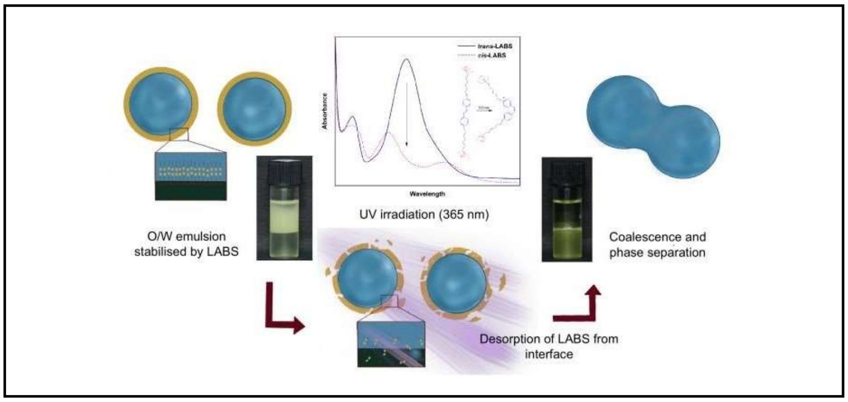

Figure 1: Graphical abstract: depicting the destabilization phenomena of oil in water emulsions using UV-light.

References

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EF-O1

Novel way to design Pickering emulsions with partial droplet coverage

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In the present work we have demonstrate engineering of Pickering emulsions of partially covered droplets by tuning particle wettability in-situ and adhesive force. The surface of hematite particles is modified with oleic acid in-situ in water - decane system. Without oleic acid, emulsion with full coverage is observed while, with addition of small quantity of oleic acid emulsions with partial coverage are obtained (fig.1 (a-b)). Further increase in oleic acid results in full coverage. The occurrence of full coverage is obvious due to mechanical stabilization as reported already [1], whereas partial coverage is rarely explored feature of system. Thus, the mechanism of these emulsions stabilization is investigated, it has been found that, the partially covered droplets are bridged together by particle monolayer and separated by a thin layer of water (fig.1 (e-f)). The bridge can be formed up to certain particle wettability, i.e droplets can be separated by water layer till particles surface goes < 50 % decane side. Interestingly, another key observation is made that particles are present at the touching point of the bridged droplets only, even then the emulsions are stable. Hence, role of adhesive forces is explored by stretching decane droplet (without /with oleic acid) after attaching to the particle-laden water-decane (without /with oleic acid) interface. It has been found that the droplet shape changed remarkably with oleic acid (73 %) compare to the without oleic acid (40 %) (fig.1 (c-d)), which is analogous to the adhesive forces. This outcome infers that the emulsions with sparse coverage are mainly stable due to strong adhesive forces between bridged droplets. Additionally, the effect of particle concentration on emulsion stability and reversibility of sparse coverage of emulsions after destabilization at high energy is studied.

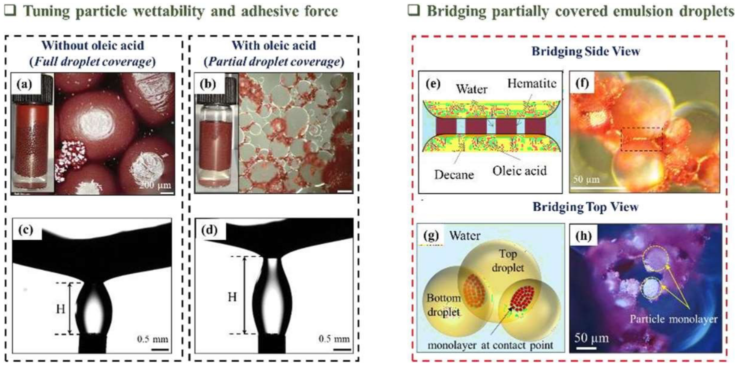

Figure 1: Emulsions with full (a) and partial coverage (b) and images captured after stretching decane droplet from the particle-laden interface without (c) and with oleic acid (d). The top view and side view of emulsion droplet bridging is shown from (e-h).

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EF – O5

A simple pathway to fabricate water-in-water emulsion-filled gels

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We demonstrate a simple yet straightforward method to produce water-in-water (w/w) emulsion-filled gels using nanoparticle-stabilized emulsification [1]. The process utilizes commercially available Ludox grade silica nanoparticles (HS-40) to stabilize the w/w emulsions formed by mixing two thermodynamically incompatible aqueous polyethylene oxide (PEO) and dextran solutions. W/W emulsion, a classic example of aqueous two- phase systems (ATPS), is preferred when using oil-sensitive drugs or other substances known to cause harmful effects, making it a suitable alternative to oil-based emulsions. Here, we show that the production of emulsion-filled gels can be influenced by the molecular weight and storage time following the “active-filler-particles (AFP)” arrangement (Figure 1). This arrangement is investigated using a state diagram developed through brightfield and fluorescent microscopy. Further, we demonstrate that the increase in the molecular weight of PEO in ATPS increases the w/w emulsion droplets’ stability owing to the synergistic effects of PEO and nanoparticles. Furthermore, the rheological studies of the emulsion-filled gels provide insights into their temporal evolution, with properties such as viscosity correlating directly with storage time, molecular weight, and composition. Intriguingly, the emulsion-filled gels generated displayed 90-day storage stability. This outstanding stability opens up various applications in low-fat food colloids, edible gels, scaffolds for tissue engineering, and porous materials.

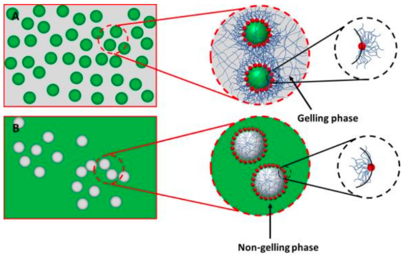

Figure 1: Schematic illustration describing the mechanism of generating different emulsion structures. A) Emulsion-filled gel (AFP) and B) Particle-stabilized emulsion.

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EF-P1

Drop Interfaces Interaction Under Application of Electric Field: Effects of Surfactants and Polymers

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The presence of polymer and surfactant in the emulsion, resulting from enhanced oil recovery techniques, poses a challenge in breaking down the emulsion. Adding surfactant and polymer changes the interfacial properties between the water and oil interface. Drop–interface interaction under an electric field is relevant in commercial desalters where in water droplets suspended in oil coalesce under an electric field, move down under gravity, and eventually coalesce with the water pool at the bottom of the desalter. This work shows that a critical electrocapillary number can describe the transition from coalescence to partial coalescence and depends on the surfactant and polymer concentration. However, a transition occurs from partial coalescence to non-coalescence after a critical electric field.

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EF-P3

Preparation of Pickering Double Emulsions by In-situ Particle Surface Modification

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[2] Polymer Engineering and Colloid Science (PECS) Laboratory, Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, India - 600036.

The petroleum industry frequently produces crude oil in the form of solid-stabilized W/O emulsion. Along with the natural surfactants in crude oil, colloidal particles such as asphaltenes, resins, and wax adsorb at the oil-water interface and create a rigid interface. Specifically, to comprehend the destabilization of wax-stabilized W/O emulsion, in waxy crude oils, it is critical to investigate the resistance coalescence process. So far, studies on the coalescence phenomenon have been done in model oils through optical observations using a high-speed camera due to the opacity of the crude oil to visible light. Therefore, to understand the water droplet coalescence at the crude oil-water interface, the present study has been done through "the Drop Rest Setup", using a Near-Infrared Camera (NIR). This setup offers the advantage of performing systematic measurements of a single droplet-interface interaction and yields the drop rest time distribution in the presence and absence of different surfactants. The drop rest time is the amount of time a droplet pauses at the interface before coalescing with the mother phase below. A broad rest time distribution was observed in a study of 90 droplets conducted in the presence of surfactants. This is attributed to the stochasticity associated with the nonuniform thickness of the interface, which gets altered by the addition of surfactants. The statistical model presupposes that a "third phase" at the interface prevents the aqueous drops, resting at the interface, preventing the coalescence of the aqueous droplet with the brine below. It is assumed that the interface is covered with a wax layer that is made up of interlinked wax particles. In the absence of surfactants, the adhesion between the adjacent wax crystals is sufficiently strong to prevent drop coalescence, except at very high temperatures. Based on these concepts, an analytical model for the distribution of rest times is suggested. The model explains the results of our experimental work.

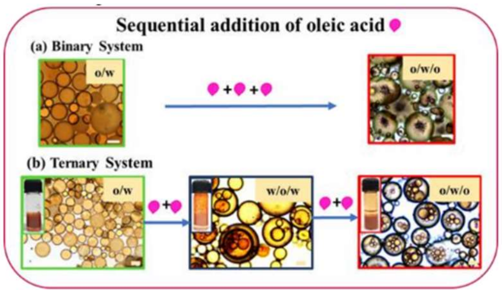

Figure 1: Emulsions stabilized by sequential addition of oleic acid in binary system (a) and ternary systems (b).

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EF-P4

Evaporative Phase Separation in Polymer Micro-droplets with Confinement and Internal Flow

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Evaporation of pure and colloidal sessile droplets1-3is a field, that we have an extensive understanding about, but in case of multicomponent drops less research has been done. The evaporation of such drops can initiate a process called liquid-liquid phase separation (LLPS). Liquid–Liquid Phase Separation (LLPS) is a special form of phase transition by which one homogeneous solution spontaneously separates into two distinct immiscible liquids, or “phases”: a dense phase, and a dilute phase. Here, we evaporate a cluster of aqueous microdroplets produced using microfluidic emulsification and show the presence of strong thermal Marangoni flows directed towards the apex of the micro-droplets. We use this system to perform LLPS in a confined environment with convective flows. The internal flow helps polymer nucleations to coalesce and grow near the droplet apex, quickly forming distinct polymer phases. It occurs even with polymer combinations that do not form distinct phases in sessile droplet evaporation. Our method of evaporation of the droplet cluster may facilitate studying LLPS in confined environments and have implications for understanding LLPS in biological systems.

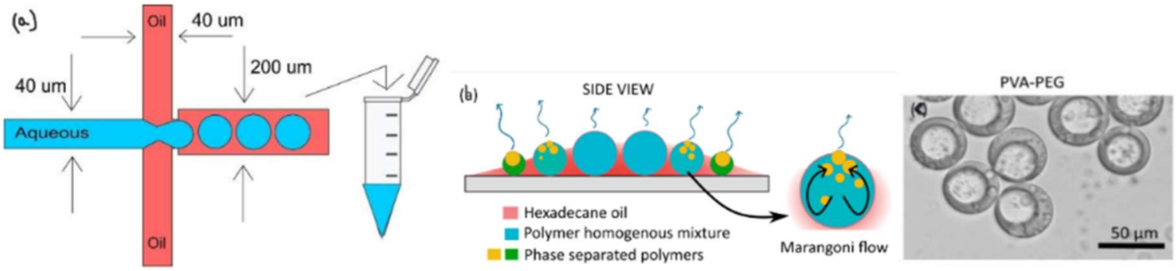

Fig. 1 (a) Microfluidic chip for producing emulsion droplets (b) Side view illustration of the emulsion droplet cluster. Evaporation (indicated by curvy arrows) results in the phase separation of the homogeneously mixed polymers. At t = 0, all the microdroplets have the same size. Droplets towards the cluster edge are only partially immersed in the oil layer. Thus, they evaporate quickly (thus smaller size) and phase-separate. (c) Evaporation of microdroplets in the emulsion produces well-separated two distinct phases of polymers.

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EF-P5

Numerical simulations of instability in Pickering emulsions caused by a mutually soluble solute

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Pickering emulsions are stabilized by solid particles rather than classical surfactant molecules [1]. They are typically more stable than conventional emulsions [2]. But for some applications, it is desired to induce instability in Pickering emulsions to extract the individual phases from the emulsion. Examples are enhanced oil recovery of crude oil (W/O system) where the oil-water separation is required and the food processing industry, for instance, extraction of milk solids. There are different techniques to induce instability in Pickering emulsions such as centrifuging, heating, and shearing/squeezing to break the droplets [3]. But these are all energy-intensive techniques, so, a novel technique that consumes less energy for destabilizing Pickering emulsions is needed. One such technique is the addition of mutually soluble solutes to induce interfacial turbulence in the Pickering emulsion system [4].

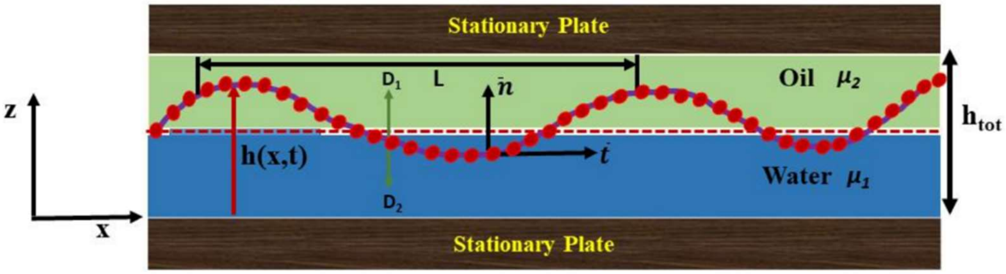

Fig. 1: Schematic representation of the problem set-up

In our work, we model the problem of mutually soluble solute transfer across two thin film phases as shown in Fig.1.

The governing equations are momentum, mass conservation, and mass transfer (convection-diffusion) equations. The commercial package- COMSOL Multiphysics software is used to solve the system of coupled PDEs to determine the effect of the mutual diffusion of solute in both phases on the stability of Pickering emulsions. Moreover, we can also determine the effect of viscosity ratio (μr), the large differences in kinematic viscosity and solute diffusivity between the two phases, the absence of surface-active agents, etc. on

Keywords: Pickering Emulsions, Hydrodynamics, Interfacial Instability, COMSOL Multiphysics, Oil Recovery

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EF – P6

Controlled Phase Inversion of Pickering Emulsions via Particle Surface Engineering

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In this work, a systematic investigation of phase inversion of emulsions stabilized by ellipsoidal particles is carried out. In particular, we consider the role of surface modification of particles and their dispersibility in different phases in the context of phase inversion. In our experiments, we model monodisperse hematite ellipsoids and modify their surface differently by oleic acid treatment. The effect of the oil-water ratio on the formation and stability of solid stabilized emulsions is studied by considering (i) particle-laden aqueous phase and oil, (ii) water and particle-laden oil phase, and (iii) particle-laden aqueous phase and particle-laden oil phase. Interestingly, when homogenized with oil, aqueous dispersions that contain unmodified hematite ellipsoids did not show any phase inversion when the oil-water ratio was varied. On the other hand, the oil phase is dispersed with hematite ellipsoids whose surface is partially modified inverse from o/w to o/w/o, and their phase inversion point depends upon on oleic acid treatment of the particles. Fully modified with oleic acid, when homogenized with water, exhibits catastrophic phase inversion. Moreover, when aqueous dispersions with pristine hematite ellipsoids and oil phases containing fully modified hematite ellipsoids are emulsified, a phase transition from o/w to o/w/o to w/o is observed as the oil-water ratio is varied. The main findings of our work are that the oil-to-water ratio at which phase inversion occurs can be tuned by particle surface modification and by dispersing particles in different phases used for emulsification.

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EF – P8

Breaking the Mold: A Novel Approach to Evolving Drop Breakup Functions and Rates Based on Multi-Physics Mechanisms in High Shear Mixers

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Process industries manufacturing food, pharmaceutical, and cosmetics products involve an emulsification step in mixers. Drop breakup in these units occurs in complex flow fields generated when fluids pass at high velocities through narrow clearances at high shear rates (>20000 s-1). During this process, the size distribution of dispersed phase, crucial in controlling emulsion property, evolves over time. The quantification of evolution in the droplet size distribution is facilitated through Population Balance Equations (PBEs) framework. Breakup rates and the associated daughter size distribution function, collectively termed as breakage functions, are needed to solve PBEs. These breakage functions constitute phenomenological formulations that encapsulate the underlying physics governing droplet fragmentation in complex flow regimes. The challenge lies in extracting these breakage functions from transient data of drop size distribution. This extraction process, known as the inverse problem, hinges on identifying self-similar patterns in the data. However, this approach encounters limitations in scenarios where self-similarity is absent. The final size distribution is a result of various drop breakup mechanisms operating parallelly. We introduce "basic modes" of breakup characterizing each of these mechanisms by a variation in dominance in each. Setting our work apart from existing research, these modes offer a more comprehensive insight into the intricate droplet fragmentation mechanisms at play. To mathematically represent the basic modes, we design robust models for their associated breakage functions. Genetic algorithm is employed for parameter estimation. A captivating phenomenon observed in high shear mixing scenarios is the transformation of an initially monomodal droplet size distribution into a bimodal configuration. This intricate behaviour defies facile prediction using conventional breakage functions. However, our novel models exhibit promise in comprehending and depicting such intricate scenarios as shown in figure below.

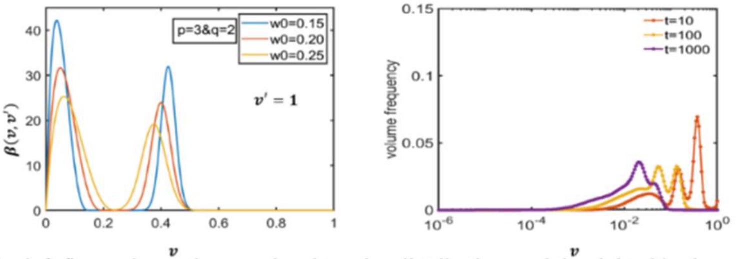

Fig. The left figure shows the new daughter size distribution, and the right side shows very different kind of size evolutions over time produced using the new breakage function.

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Oil in water Emulsion Stabilized by HEUR Polymers

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Abstract: -

The majority of polymeric emulsifiers include hydrophilic and hydrophobic domains and are composed of di and triblock copolymer moeity. In this work, we show that hydrophobically modified hydrophilic homopolymers (hydrophobically modified ethoxylated urethane/HEUR) can be effective stabilizers of oil-in-water emulsions. We synthesize HEUR polymers by functionalisation of polyethelyne oxide(PEO) with alkane chain using isocyanate linkers through condensation reaction. Using HEUR homopolymers and n-decane as model non-polar phases, we show that even lower molecular weight polymers can stabilize emulsions over several weeks with minimum concentrations. We highlight the role of alkane chain attached to the polyethylene oxide on the stability of emulsions, through comparison of emulsion stability with and without alkane chain on PEO. This study demonstrates that modifying the water-soluble homopolymers with hydrocarbon end-groups can drastically increase the stability of emulsion.

Key words: - ***HEUR Polymers, Emulsion, Electronic microscopy, Interfacial tension.***

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Application of Empirical and Fundamental Rheology to understand the wheat flour and non-wheat flour Dough properties and its relationship with end products

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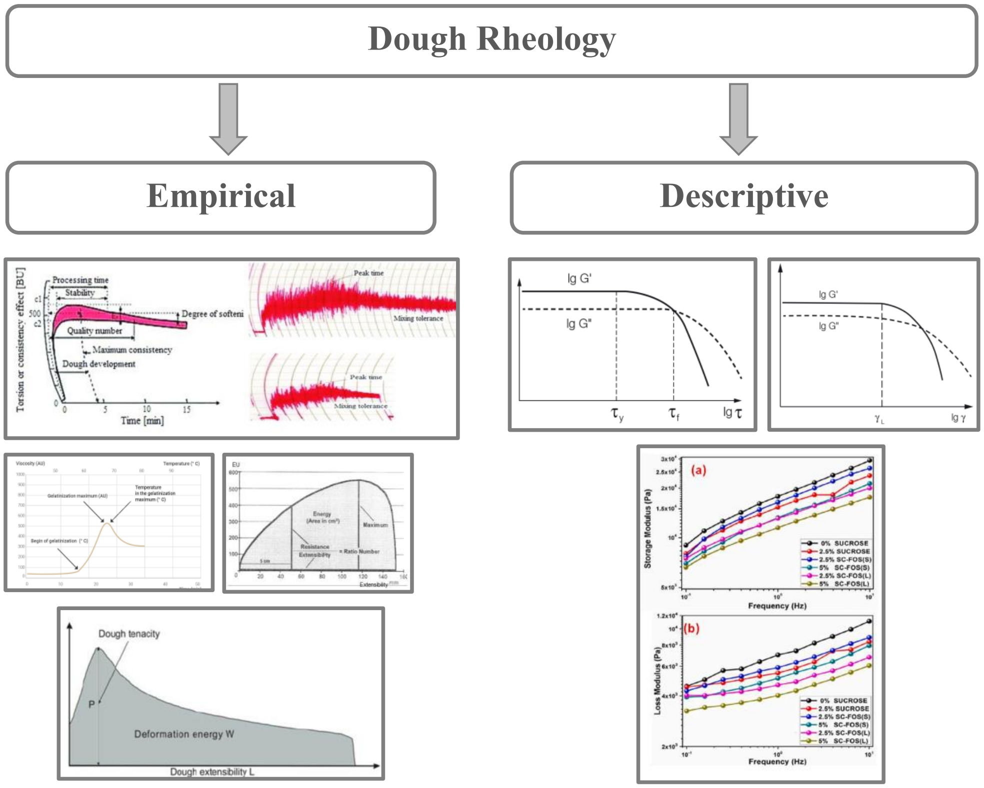
Abstract

Understanding dough rheology is important for the effective production of food products. In food industry, rheology helps in product formulation and optimization, quality control, process development and scale up. Rheological properties are necessary to analyse the dough behaviour during mechanical handling and its effect in the quality of the finished product. Knowledge about rheological behaviour and instruments is important as automation in food industry is growing at rapid pace. Empirical rheology instruments such as Farinograph and Mixograph records and measure the resistance to deformation of a flour or dough; amylograph provides the alpha-amylase enzyme activity in flours and it stimulates the process inside a bread crumb during baking process; Alveograph measures the resistance of a bubble in dough to expansion; Extensograph measures the flour quality and dough stretching behaviour. Fundamental rheology instruments such as rheometer measures the flow and deformation behaviour of the materials. In food systems, rheometer can be used to measure the viscoelastic behaviour, and stress-strain relationship etc., Different types of rheometers are available commercially. The dough will experience various stresses and deformation at various stages of the process. The gluten network is responsible for its unique viscoelastic properties. The formation and the sstructure of the gluten network depends on all the processes that a wheat flour and wheat dough undergoes such as dough mixing, kneading, sheeting and other similar mechanical actions. In a rheometer, the oscillation tests like amplitude sweep, frequency sweep, temperature ramp, creep and structure recovery tests are performed which can closely mimic the realistic processing conditions of dough and support in deciding the optimum processing parameter to obtain a desirable baked product. A sinusoidally oscillating deformation of known magnitude and frequency is applied on the dough, the outcome is measured as a phase lag angle between stress and strain that further provides the storage modulus (G’) and loss modulus (G") which represents the elastic and viscous components respectively of the dough which can be co-related to the structural changes in the dough due to

the intensity of processing conditions and during baking. The starch gelatinization is a significant part of baking, the progress of starch gelatinization due to the increasing temperature can be observed in the graphs of storage modulus during a temperature sweep test. Thus, the Empirical and Descriptive Rheometry inflict high deformation forces which provides an output in terms of relative units that can be used to study the dough processing and baking behaviourur. In this talk, various empirical and fundamental rheological instruments used to measure the dough behaviour will be discussed in detail.



Food science – A soft matter perspective

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Abstract

Colloid science plays an important role in preparation and development of food products. Several phenomena such as emulsification, foaming, gelation, nucleation, vitrification, glass transition etc play a vital role in determining the food processing conditions. Thus, from a physics point of view, food can be understood as a soft material with complex multiscale structure. In my presentation, I will briefly discuss about the important physical phenomena that one can observe in food processing and I will address two key problems that my research group is currently working on viz. Emulsification of highly concentrated Pepper oleoresins for design of retail flavouring products and application of cold plasma technology to enhance techno-functional properties of plant based proteins for food product applications.

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Application of twin-screw extruder for protein texturization: Interplay of system & process parameters on product properties

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Abstract

Proteins are one of three macronutrients in our diets and nutritional recommendation has been to consume 0.8g protein per kg body weight per day which leads to 175 billion kg global protein requirement per year. The emerging muscle-centric view of health puts doubles the daily requirement to 1.6g protein per kg body weight per day or 375 billion kg global protein demand. Dense protein foods such as animal meat, dairy and legumes are increasingly being sought after to meet the protein needs. While plant-based protein dense foods have a much lower environmental footprint and efforts are on globally to increase their use in global diets as one of the pieces to address global warming, they are incomplete in essential amino acid profile, have lower digestibility, and have taste and texture profiles that are not always preferred by a wider population, making their adoption in daily diets difficult.

This has led to endeavors to develop plant-protein based food products that address the above challenges, and one approach has been to create textured proteins, with clean tastes, good amino acid profile and higher digestibility for applications in various foods such as (soy) 'chaap' and meat analogues. Various technologies are being explored to produce textured plant-based proteins of which the twin-screw extruder coupled with heating or cooling dies has proved to be the most scalable. The final texture is a result of the interplay of ingredient composition, system parameters and process parameters.

In this talk we will talk about our extrusion experiments on blends of soy proteins and millet flours and efforts to study the effect of system and process parameters on product textural attributes by using rheology, FTIR spectra and targeted protein solubility to understand the protein-protein interactions that create the fibrous structures during the texturization process.

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Emerging trends on formulations of bigels, their rheological characterization and correlation to food applications

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Biopolymer-based gel systems are being explored in recent times for a wide range of industrial applications ranging from food to pharmaceuticals to cosmetics. Hydrogels, oleogels, emulgels and bigels are some of the gel-based systems that are classified based on the dispersed phase. Hydrogels are majorly fabricated using proteins, polysaccharides, or their composites. They exhibit excellent water solubility, water holding capacity and swelling behavior. However, hydrogels cannot effectively encapsulate lipophilic compounds. Several pharmaceutical formulations which target the delivery of bioactive compounds through the lipophilic barrier of the skin require solubilization of lipophilic compounds in the delivery system. Furthermore, fat-replacement and reduction in foods still remains a great challenge, wherein mimicking the textural and rheological properties of foods is of utmost important. Emulgels pose as a solution to the problem. The emulsification of the oil-rich phase at the hydrogel-emulsion interface facilitates the delivery of both hydrophilic and hydrophobic bioactive compounds. However, emulgels often exhibit phase separation. Oleogels are soft structures wherein the continuous liquid phase is oil and/or fat, and require structuring agents or oleogelators such as waxes, fatty acid derivatives, and phytosterols to form an interconnected entangled network while cooling. Bigels comprise of a special category of hybrid gels comprising of a hydrogel and an oleogel fraction which confer it both hydrophilic and lipophilic characteristics. The rheological properties of the bigels can be tailored by varying the ratio of the hydrogel and the oleogel in the formulation. These properties of the bigel deeply impact the swelling and release properties. Therefore, optimization of the bigel formulation is undertaken on the basis of rheological profile. Since they are often expected to replace fats, the melting behavior is also estimated by the temperature ramp experiments. The type of oleogelator and the hydrogel matrix directly impacts the rheological and textural profile of the bigel. Depending on the hydrogel/oleogel ratio, the bigel system can be a hydrogel-in-oleogel or oleogel-in-hydrogel system. This presentation looks in to the fabrication of different bigels, their rheological characterization and its correlation to food applications. A couple of case studies conducted in our laboratories are also presented.

Indian Society of Rheology

Recent Research Developments & Future directions in Food Processing

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Abstract

Food is a complex matrix with various components such as moisture, proteins, fats, carbohydrates, vitamins etc. and hence it makes Food Processing also complex. Further unlike chemical products, food product is for human consumption. So special attention is to be paid for maintaining microbial quality (food safety) and sensorial quality while retaining the nutrients.

Furthermore, as moisture content vary during processing, product shrinkage occurs and as a result, all the physical and thermal properties such as density, porosity, and mass and thermal diffusivities no more can be assumed to be constants during mathematical modelling. Chemical engineering has a lot of similarity with the food processing in terms of unit operations. To make food processing more Cost and Quality effective, there is a need for Innovation and Intelligent ways and means of processing. The talk presents in detail the reasons for such a need, examples of several innovations and a few case studies highlighting the intelligent application of chemical engineering principles to food processing citing current and future activities at IIT Tirupati in collaboration with a wide cross section of expertise available within our institute and outside.

Rheological study of cereal based fermented food suspensions

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Abstract

Cereal based fermented (or ‘aerated’) food products have been an integral part of the diet in many parts of the world. Fermented foods receive worldwide attention owing to their disease-preventing and health promoting effects in addition to reduced cooking time, improved flavor, appearance, nutritional value and storage stability. Fermented suspensions made from rice and blackgram are very popular in South-East Asian countries as several culinary items, such as, Dosa, Vada, Idli, etc. The cereal batters essentially consist of starches and proteins which undergo changes/ modifications with time of preparation and during processing that ultimately affect their flow characteristics. Starch gelatinization and protein denaturation are the two mechanisms that play crucial role in heat induced changes. It is essential to comprehend the suspension behaviour under varied conditions of processing and storage. A knowledge of the rheological properties of such suspensions is important for the assessment of batter quality characteristics during and after cooking like spreadability, texture, consistency and firmness. In the present study, the changes in rheological properties of ‘Dosa’ and ‘Vada’ batters with sample characteristics (ingredient type, composition, particle size and solid concentration) and processing conditions (time and temperature) are investigated. This will involve fundamental understanding of structural transformations at various stages of batter heating and how various biochemical changes during cooking of such batters affect their viscoelastic behaviour.

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FS-P1

Rheological characterization of composite hydrogels fabricated from pea protein and konjac glucomannan

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Plant-based hydrogel systems are being explored in recent times for their several prospective applications in food systems. In this study, a composite hydrogel consisting of pea protein and konjac glucomannan (KG) was fabricated using three different gelation approaches, namely neutral gelation, salt-set gelation and alkaline gelation. Hydrogels from sole pea protein were made by the pH-shifting method; but were brittle and weak. The addition of KG improved the elasticity of the pea protein hydrogels, which was evident from the creep recovery and structural recovery data. The highest cross-over and yield strain values were obtained for alkaline-set hydrogels; thereby indicating the highest resilience to strain.[1] Thixotropicity was found to be less pronounced for salt-set hydrogels. The rate of re-entanglement of the hydrogel network was higher for SO_4^{2-}-induced gels than the Cl^--induced gels. The SO_4^{2-} had a greater positive effect on the structural recovery than Cl^-; which can be attributed to the greater salting-out effect of the sulphates.[2] The consistency coefficient (*K*) and flow behavior index (*n*) exhibited an increase and decrease, respectively with the addition of KG; indicating the formation of an interconnected structure with limited mobility of the biopolymer chains. The hydrogen bonding between the unfolded pea proteins and KG were one of the stabilizing forces in the sols; which were broken during the initial stages of heating (20-60 °C). A rapid and a sharp increase in *G'* and *G"* soon after, indicated the predominance of hydrophobic interactions towards the aggregation of the biopolymers; thereby facilitating the sol-gel transition.[3] The infrared spectra of the hydrogels revealed a change in secondary structure of proteins due to the addition of KG.

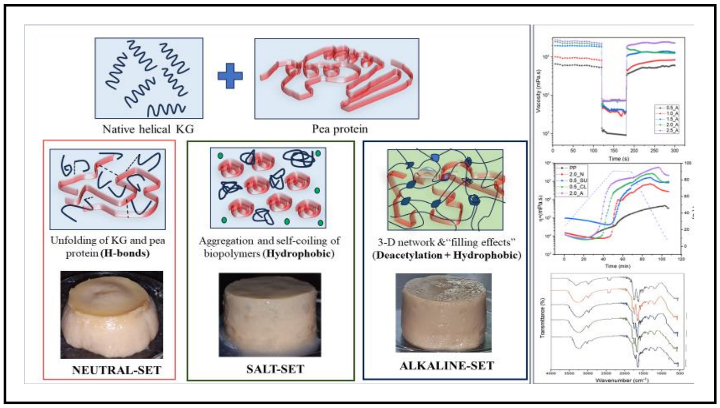

Figure 1: The different schemes of gelation and the predominant interactions between the protein and glucomannan affecting the rheological properties of the composite hydrogels.

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A bottom-up understanding of the rheological and microstructural characteristics of edible oleogels

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Today, increased consumption of saturated and trans-fat is causing concern due to its adverse impacts on health, including obesity and cardiovascular diseases. As a result, more research is being done on healthy fat replacements that involve transforming vegetable oils into oleogels without changing their chemical properties, which lowers saturated fats and eliminates trans-fats. In this study, mono, bi, and ternary gelator mixes of plant waxes, monoglycerides, and stearic acid were used to make oleogels from sesame oil, groundnut oil, high oleic sunflower oil, and coconut oil. Oleogelation resulted in the formation and branching of crystals, that form aggregates which interact with each other through hydrogen bond and van der Waals forces. Thus, the immobilization of liquid oil in the three-dimensional network structure minimized the void spaces between the crystals and thereby improved the mechanical strength with oil binding capacities above 95%. The microstructure of monoglyceride oleogels revealed needle-shaped crystals, and higher levels of monoglycerides produced a densely packed, evenly aligned network that provides oleogels a stronger structure. On the other hand, ground nut oil oleogel made of binary gelator blends (β-sitosterol and monoglyceride) displayed self-assembled fiber-like structures, reflecting that gelators retained their distinct crystalline structure. Additionally, confocal laser scanning microscopy images confirmed that the concentration and composition of fatty acid / gelator alters the morphology of oleogels. Moreover, the thermoreversible behavior of oleogels was confirmed through *in-situ* hot stage microscopic analysis. Rheological characterization revealed that the magnitude of elastic modulus was remarkably greater than viscous modulus, suggesting that all the oleogels had solid-like properties, which are characteristic of gels. The higher G' values specify the increase in gelator concentration, which enhanced the mechanical stability and further resulted in highly structured oleogels. Collectively, the obtained results suggested that it is possible to create solid fat alternatives using edible oil, which can mimic the characteristics of plastic fat. This will pave the way for the production of healthy food products to promote health benefits through straightforward oil structuring techniques.

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FS-P3

Formation and characterization of polysaccharide-based oleogel derived from emulsion: A Rheological Investigation

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Oleogels are structured edible oils developed as an alternative to the conventional solid fats to reduce the intake of saturated and trans-fats that are considered to have a negative impact on human health. In this study, the oleogel was prepared with an emulsion template approach. The electrostatic interaction, hydrogen bond cross-linkages and Schiff base reaction were the primary factors between the chitosan, vanillin and multi-source edible oil for the formation of stable oleogels. These parameters play a crucial role in formation of a stable three-dimensional network that immobilizes the liquid edible oils within a solid framework, resulting in a gel-like consistency. In addition, lipophilic bioactive molecule (phytosterols) was added in two different concentrations of 2.5% (OG-2.5) and 5% (OG-5) in the lipid phase of the emulsion to enhance the nutritional value of the oleogel and the food products. The microstructural characterization of oleogels confirmed the formation of a complex network between chitosan and vanillin / phytosterol, leading to the entrapment of oil within the gel structure. The FTIR spectrum showed minor peaks at 1664 cm^{-1} in OG-2.5 and 1652 cm^{-1} in OG-5 could be attributed to C=N vibration characteristic of imines indicating the schiff base reaction between the amino group from chitosan and aldehyde from vanillin. The rheological characterization of both the oleogels consistently showed G' > G" indicating solid-like behavior, the flow behavior of the oleogels was found to be shear thinning, apparent viscosity extremely decreased as the shear rate increased from 0 to 100 s^{-1}, the study examined the thixotropic behavior relative to time and the extent of structure recovery. The measurements revealed close to 90% recovery from the applied forces, evident of a reversible and elastic gel network [1]. As a result, these oleogels can serve as viable alternatives to conventional solid fats in a wide range of food applications.

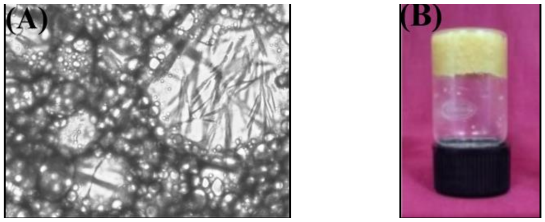

Figure 1: (A) Brightfield microscopy images at 100*x* magnification of the emulsion after crosslinking & (B) Oleogel.

Reference

[1] Thomas, P. E. (2023). Original article Virgin coconut oil oleogel: gelation mechanism, rheological, structural and thermal properties. 1434–1443. https://doi.org/10.1111/ijfs.16305

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FS-P4

Study on Evaporation of Liquid Sugarcane Juice Droplet for Granular Jagerry Production

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India is the largest producer of jagerry with contribution of about 70% of the total jagerry production in the world. However, there are some major constraints in jagerry export mainly due to unorganized production based on conventional methods and the absence of standard protocol, automation and packaging standards. It is imperative that modern processing technology is adopted along with detail understanding on the sub-processes to improve the scenario. In this context the application of the spray drying technology for granular jaggery production can be explored since it has the potential to address almost all the abovementioned constraints. For instance, a key advantage here is the significant improvement in the storage ability of the granular powder compared to solid jagerry. Although the spray drying is a well-established process, there is as such no standard for granular jagerry production. In such case, the atomization of the sugarcane juice and evaporation of the liquid droplets are crucial stages for achieving the desired quality of the granular jagerry powder, and the liquid temperature plays a critical role in both the above processes. In this work we focus on the evaporation of a single sugarcane juice droplet, the understanding of which is central to the success of the spray drying process. The sugarcane juice is preheated to different temperatures, and for each case a known volume of the liquid is loaded at the center of a cross-wire arrangement, as a droplet using a micro-pipet. The droplet evaporation process is imaged using a camera. The images are analyzed to obtain the time evolution of droplet size. For instance, when the juice is heated to 100ºC, the droplet size does not vary much though the solidification process continues. The Scanning Electron Microscopy (SEM) analysis will be performed to examine the particle morphology. The experiments will provide insight into the role of liquid preheating on the evaporation process of the sugarcane juice droplet and the particle quality.

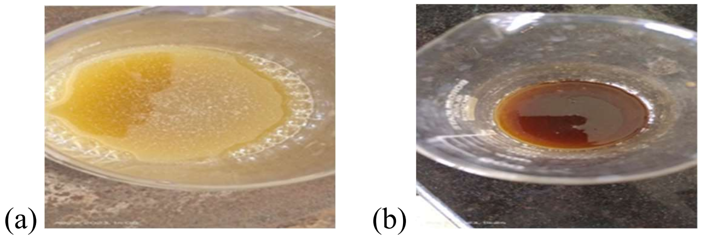
(a) (b)

Figure 1: (a) Fresh Sugarcane Juice at room temperature of 36ºC,(b) After heating to 100ºC(concentrated).

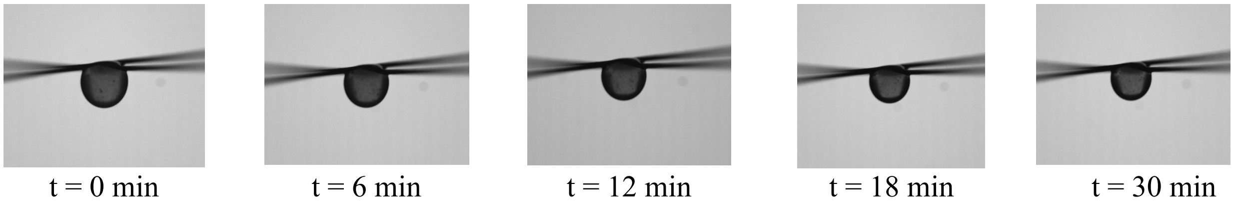
t = 0 min t = 6 min t = 12 min t = 18 min t = 30 min

Figure 2: Time sequence of images of sugarcane juice droplet with initial temperature of 100ºC.

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FS – P5

Unveiling Rheological Transformations in High Moisture Extrusion: Bridging Insights from Raw Material to Extruded Meat Analogues

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Abstract

The process of high moisture extrusion transforms soy protein isolate – millet flour blends into fibrous textures, making it crucial to understand the rheological changes occurring during extrusion and in the resulting product. This study aimed to investigate the rheological transformations within raw material blends under extrusion like conditions and to characterize the viscoelastic properties of the extruded high moisture meat analogue (HMMA). Utilizing a closed cylinder (referred as pressure cell) for measurements under simulated extrusion conditions. The study revealed substantial changes in viscosity and viscoelastic properties during heating and cooling phases. Viscosity decreased during heating, while a build-up was observed during cooling at a specific moisture content and similar trend was witnessed in the shear modulus.

The viscoelastic properties of HMMA was measured with a profiled parallel plate. Upon reaching the linear viscoelastic region (0.33 – 2.95 % strain), a decline in G´ (elastic modulus) and a simultaneous nonlinear increase in G´´ (viscous modulus) was seen across all samples, indicating an irreversible structural change in the extrudates. With further strain increase, an intersection between G´ and G´´ marked the material's transition to flow behaviour and subsequent disintegration. Analysis using the power law model during a frequency sweep revealed a behaviour index n´ around 0.1, indicating HMMA's elastomeric characteristics. Additionally, the consistency index K´ of pure soy protein surpassed that of the blends, suggesting higher structural strength and superior viscoelastic properties. This study provides crucial insights into understanding both the extrusion process and the quality attributes of HMMA with different textures to mimic animal meat or specific parts of muscle.

FS – P6

Low Moisture Extrusion for Textured Vegetable Protein (TVP) Production from Soy and Pea Protein Isolates: System Response, Expansion Ratio and Rehydration Properties

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Abstract:

The study explores the intricacies of low moisture extrusion, a pivotal process for producing Textured Vegetable Protein (TVP) using soy and pea protein isolates. With a focus on elucidating crucial system parameters, this research emphasizes evaluating resulting product attributes while varying feed moisture content (17.5%, 22.5%, and 27.5%) at a specified temperature (150 °C). A comprehensive analysis of system parameters (including Specific Mechanical Energy, melt temperature, and pressure) and optimization strategies is presented, highlighting their influence on the production process and the quality of the obtained TVP. Notably, expansion ratios, indicative of product quality were examined, revealing increased expansion as feed moisture content decreased. Additionally, a comparison between soy and pea protein illustrated higher expansion ratios for soy protein. Furthermore, the rehydration properties crucial for culinary applications were assessed and correlated with process parameters, demonstrating consistent trends in the results. Morphological features of the produced TVP showcased through images, complement the comprehensive analysis. This investigation offers valuable insights into optimizing low moisture extrusion techniques, enhancing the creation of high quality TVP and opening avenues for enhanced applications in the food industry.

Low temperature dynamics in a model glass former

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With increasing computational power and with the use of methods for accelerated sampling, it has become possible to explore the equilibrium and dynamic properties of glass forming liquids well below the range previously accessible. I present results from long molecular dynamics simulations of a well studied model glass-former, the Kob-Andersen binary Lennard-Jones mixture, accessing temperatures well below the mode coupling crossover temperature. The dynamics exhibits a change in character, exhibiting behaviour that may be described as a fragile-to-strong crossover, with the temperature dependence of relaxation times becoming closer to Arrhenius dependence, and a saturation of measures of dynamical heterogeneity, and a change in the geometry of cooperatively rearranging clusters. One also observes an apparent deviation from the Adam-Gibbs relation between relaxation times and the configurational entropy, but a proper accounting of anharmonic contributions to the vibrational entropies leads to the conclusion that the Adam-Gibbs is indeed valid, over six orders of magnitude slow down in relaxation times.

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Fatigue Damage of Bituminous Binders using Large Amplitude Oscillatory Shear

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Fatigue is one of the primary modes of failure in a bituminous pavement. Bituminous pavement layers are composite, consisting of binder, filler, and aggregates. Understanding the mechanical behavior of bituminous layers demands investigation of their different material scales, such as the binder, mastic, and mixture scales. Of the methods used to characterize fatigue damage of bituminous materials, energy dissipation is widely used; however, it is complicated due to the presence of other modes of dissipation, such as viscous dissipation. In this talk, I present our recent work on quantifying fatigue damage using a nonlinear viscoelastic fluid model. I present the use of Large Amplitude Oscillatory Shear experiments on bituminous binders and mastics. I also discuss the use of Fourier rheology related to the same.

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On the structure-viscoelasticity relationship of reversible polymer networks

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Reversible polymer networks (RPNs) have widespread applications in self-healing materials and recyclable plastics. [1] These polymeric materials embody functional groups which can be programmed to form irreversible or reversible crosslinks through covalent, non-covalent, or dynamic covalent bonding interactions. In this work, using equilibrium Langevin dynamics simulations we understand the relationship between the structure and viscoelasticity of a dually crosslinked RPN. We employ single-chain nanoparticles (SCNPs) to model the reversible polymers and dual crosslinking, where orthogonal crosslinkers (A and B) are introduced in the polymer backbone. SCNPs are attractive polymeric materials owing to their potential applications in drug delivery and catalysis, and comparable morphologies with intrinsically disordered proteins [2].
At infinite dilution, we find that the orthogonal cross-linking leads to more compact SCNPs, suggesting an effective approach for generating globular SCNPs.[3] In addition to the structure of the chains, we explored the role of weak (A-A) vs strong bonds (B-B) in tuning the stress relaxation behavior of the networks, by systematically varying the relative composition of A monomers (x), at a concentration where the system-spanning network will form.[4] Interestingly, we find a non-monotonic trend in the diffusivity and consequently in the stress auto-correlation function of the system w.r.t. x. In addition, we find that in the plateau regime, the dynamics is dictated by the strength of the weak bonds, whereas the terminal relaxation behavior of the stress auto-correlation function depends on the strength of the strong bonds. Further, we find that the distribution of the crosslinking monomers has a significant impact on tuning the stress relaxation behavior. We believe our results aid in understanding the interplay of weak vs strong bonds and the specific effects of their relative composition and distribution in tuning the viscoelasticity of the RPNs.

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Dramatic growth of Dynamic and Static correlations in Active Glass-forming Liquids as probed via rod-like probe particles

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Activity driven glassy dynamics is ubiquitous in collective cell migration, intracellular transport, dynamics in bacterial and ant's colonies as well as artificially driven synthetic systems such as vibrated granular materials, etc. Active glasses are hitherto assumed to be qualitatively similar to their equilibrium counterparts at a suitably defined effective temperature, T_{eff}. Using large-scale simulations, we show that, in fact, an active glass is qualitatively different from an equilibrium glassy system. Although the relaxation dynamics can be similar to an equilibrium system at a T_{eff}, effects of activity on the dynamic heterogeneity (DH), which has emerged as a cornerstone of glassy dynamics, is quite nontrivial and complex. In particular, active glasses show dramatic growth of DH, and systems with similar relaxation time and can have widely varying DH. In particular, we are able to demonstrate a dramatic growth of correlation length in these systems with increasing activity which is very different compare to the passive glasses. Finally, we propose a novel method which can be implemented in experiment to measure the strong growth of dynamic heterogeneity and its associated length scale in these systems using a rod-like probe particle. If time permit, I will also discuss Stokes-Einstein and Stokes-Einstein Debye breakdown of the probe particle in these active glassy medium and their direct links to the growing dynamic heterogeneity length scale.

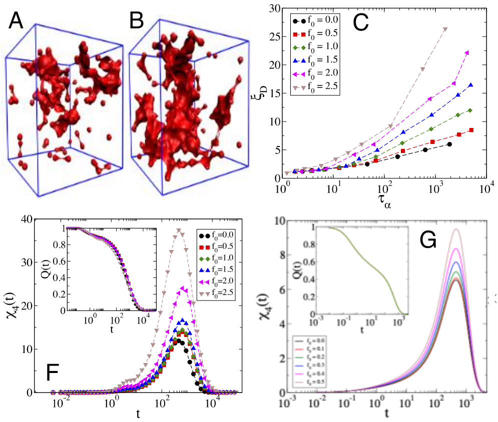

Figure 1: Dramatic growth of Dynamic Heterogeneity (DH) in active glasses and corresponding rise in dynamic correlation length.

Reference:

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3. Length-scale Dependence of Stokes-Einstien Breakdown in Active Glass-forming Liquids, A Mutneja, Smarajit Karmakar arxiv.2306.10229 (2023).

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Dynamics and structural ordering in binary colloidal-solvent mixtures of glass-formers

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We investigate the dynamics of a binary mixture comprising colloidal particles dispersed in a solvent of smaller-sized particles, revealing a transition from ternary to an effective binary system. Through meticulous analysis of effective potentials and pair correlation functions, our study unveils cooperative reorganization clusters (CRCs) in which localized particles from enduring nonchemical bonds with a central particle, thereby impacting relaxation dynamics. The manipulation of solvent concentration is found to intricately influence microscopic structural order and CRC size, consequently dictating the glassy dynamics that range from fragile to strong behaviors. Our findings emphasize CRCs, identified through static pair correlation functions and inherent fluctuations, as sole players in the complex realm of glass transition physics.

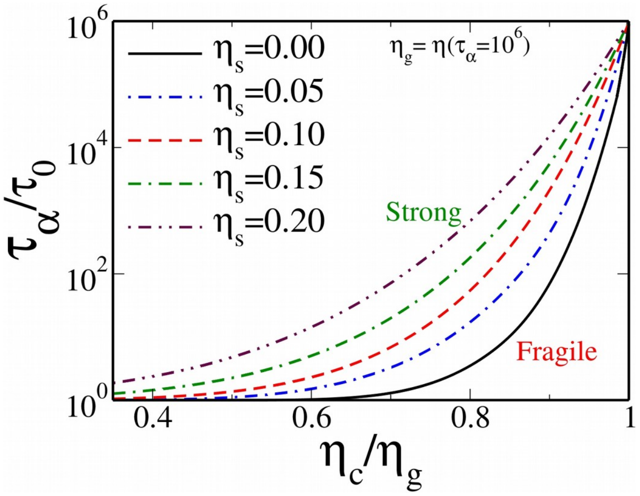

Figure 1: Angell plot of relaxation time as a function of normalized packing fraction at different solvent packing fractions η_s. At lower η_s, the relaxation time exhibits a sharp growth upon increasing η_c, i.e., a feature of a fragile glass former, whereas at higher η_s, the relaxation time display relatively slow growth with, suggesting a strong glass former.

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Inter-particle adhesion induced strong mechanical memory in a dense granular suspension

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Repeated/cyclic shearing can drive amorphous solids to a steady state encoding a memory of the applied strain amplitude. However, recent experiments find that the effect of such memory formation on the mechanical properties of the bulk material is rather weak. Here we study the memory effect in a yield stress solid formed by a dense suspension of corn starch particles in paraffin oil. Under cyclic shear, the system evolves towards a steady state showing training-induced strain stiffening and plasticity. A readout reveals that the system encodes a strong memory of the training amplitude as indicated by a large change in the differential shear modulus. We observe that memory can be encoded for a wide range of training amplitudes both above and below the yielding, albeit, the strength of the memory decreases with increasing amplitude. In-situ boundary imaging shows strain localization close to the shearing boundaries, while the bulk of the sample moves like a solid plug. In the steady state, the average particle velocity inside the solid-like region slows down with respect to the moving plate as the training strain approaches the training amplitude, however, as the readout strain crosses the training amplitude, the average particle velocity suddenly increases. We demonstrate that inter-particle adhesive interaction is crucial for such a strong memory effect. Interestingly, our system can also remember more than one input only if the training strain with a smaller amplitude is applied last.

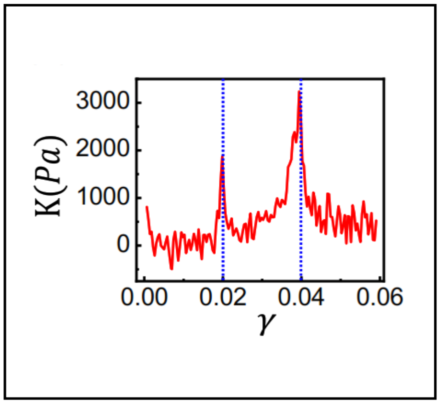

Figure 1: Multiple memory formation in a granular gel.

References

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A Curious Case of the Thixotropic Timescale

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Thixotropy is characterized by an increase in viscosity when a material is subjected to no flow (quiescent) or weak flow conditions and a decrease in viscosity when it is subjected to strong flow conditions. It has been observed that many soft glassy materials that include colloidal gels and glasses show thixotropic characteristics. Lately, there has been renewed interest in thixotropy and the characteristic timescale associated with the same known as thixotropic timescale. In this presentation, we will discuss the various meanings attributed to thixotropic timescales in the literature, as well as the inherent contradictions associated with them. It is suggested that a thorough understanding of thixotropic materials, along with an analysis of experimental observations, is necessary in order to establish a meaningful definition of thixotropic timescale. Finally, we present an approach that identifies critical characteristics of the thixotropic timescale and provides limits and bounds on the same. We feel that this proposed approach has important implications for mathematical modeling of thixotropic materials.

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Indian Society of Rheology

Nature of universal subdiffusion crossover in molecular glass-formers

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The issue of diffusion in supercooled liquids and glasses is a key element in understanding glass transitions. These materials don't follow typical Brownian motion principles, such as linear time-dependent mean-squared displacement and Gaussian displacement distribution. The deviations from these features depend on the scales considered and lead to shifts between different diffusion mechanisms. Universally, molecular/polymeric glass formers exhibit a crossover from non-Gaussian to Gaussian subdiffusion [1-2]. Despite extensive simulation and experimental work on this universality, a fundamental model hasn't been established, preventing a comprehensive picture of the underlying non-Gaussian behavior. In particular, the universal exponential tails observed as a signature in van Hove self-correlation of glassy relaxation has not been established in this non-Gaussian subdiffusive phenomena. In this work, we develop a model based on non-Gaussian fractional Brownian motion (nGfBm), extending the fBm model to incorporate non-Guassian features using a jump-kernel [2]. Employing the Fokker-Planck equation for this model, we describe the subdiffusion crossover as observed using incoherent quasielastic neutron scattering (IQENS). It is notable that the non-Gaussianity in the subdiffusion process is fundamentally driven by an exponential jump-kernel which is governed by a characteristic jump length and waiting time. By obtaining the exact solutions for the case of exponential jump-kernels, we calculated van-Hove self-correlation functions in the strongly non-Gaussian limit, as shown in Fig. 1 for pure ethylene glycol. The exponential tails in the van Hove self-correlation function are clearly evident in the non-Gaussian limit of the relaxation which is observed for $t < 20$ ps, typically waiting times in the system.

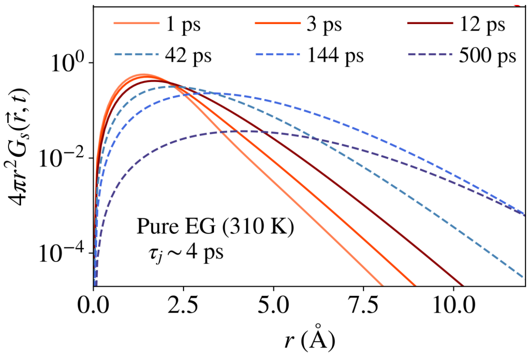

Figure 1: The radial van Hove self-correlation function calculated based on IQENS measurements on ethylene glycol (EG) at 310 K. Here τj is the characteristic waiting time between jumps in the diffusion process.

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Ion diffusion, ion-pair relaxations and viscosity of pectin-[BMIM][PF_6] electrolytes

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We investigate the effect of pectin on the structure and ion transport properties of the room-temperature ionic liquid electrolyte 1-n-butyl-3-methylimidazolium hexafluorophosphate ([BMIM][PF_6]) using molecular dynamics simulations. We find that pectin induces intriguing structural changes in the electrolyte that disrupt large ionic aggregates and promote the formation of smaller ionic clusters, which is a promising finding for ionic conductivity. Due to the presence of pectin in [BMIM][PF_6] electrolytes, the diffusion coefficient of cations and anions is observed to decrease less significantly when compared to the alterations seen in ethylene carbonate electrolytes containing pectin. However, the pectin induced changes in diffusion are observed to be consistent with the corresponding effect on viscosity and ion-pair relaxations. Our analysis shows that while there exists good correlations between the ionic diffusivities and ion-pair relaxation timescales in pectin-[BMIM][PF_6] electrolytes, the overall transport mechanisms are slightly distinct from those found in neat [BMIM][PF_6] electrolytes.

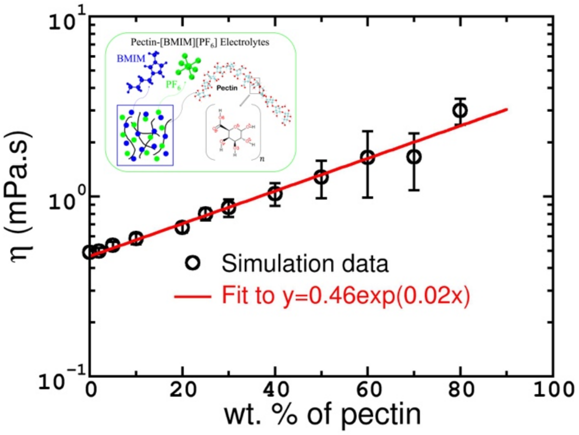

Figure 1: The average viscosity calculated using Green-Kubo approach.

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Rheology modification with polymeric loops

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Tailoring the rheological properties of soft composites at molecular level has been a thematic at the forefront of engineering research. A formidable challenge is understanding the role of macromolecular architecture on topological constraints and the resulting network dynamics. Ring polymers represent a unique case because of the absence of free ends that mediate conformational arrangements in a topological entanglement network. It has been shown that these macromolecules exhibit a power-law stress relaxation, in the absence of entanglement plateau. Here, we discuss the rheology of these loopy structures. We show that they exhibit unusual nonlinear response in shear and, especially, in extension because of loop interlocking. Adding small amounts of ring polymers to entangled linear matrices yields a reinforcement effect, which can be understood by invoking the (coherent) constraint release processes on the rings due to the escape (unthreading) of linear chains. The ring-linear molecular weight asymmetry is important and examined in this work. We also consider the addition of a few single chain nanoparticles, which are also (crosslinked) loopy structures, on linear matrices and show that, indeed they exhibit a qualitatively similar reinforcement effect, because of the action of loop threading. The punchline is the emerging ability to selectively tailor the rheological properties of a wide range of polymeric networks with loops and, at the same time, provide insights on the physics of the constraint release process.

This presentation reflects a large project in collaboration with D. Parisi, K. Peponaki, C. Pyromali (Crete), M. Rubinstein (Duke), V. Mavrantzas, D. Tsalikis (Patras), T. Chang (Pohang), Q. Huang, W. Wang, O. Hassager (DTU), T. O'Connor, G. Grest (Sandia), N. Hadjichristidis (KAUST), G. Sakellariou (Athens). Support from the Hellenic Foundation for Research & Innovation (project 4631) is gratefully acknowledged.

Dynamics of supercooled liquid in complex confined geometry

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The dynamics of a bulk liquid in its supercooled state has been investigated extensively in experiments and computer simulations and is well understood. However, much less is known about the influence of a spatial confinement on the dynamic properties of a liquid. Attempts were made to understand the influence of restrictive geometries in the form of thin films or narrow pores. Nevertheless, the effect of random complex porous confined structures on such systems is missing. In this work, we employ molecular dynamics simulations to examine the relaxation dynamics and static properties of a binary Lennard-Jones liquid confined within porous host with diverse geometric structures. Our findings reveal that the confinement strongly impacts the dynamics, resulting in highly stretched time correlation functions compared to the bulk, while leaving the system's static properties unaffected. Specifically, the relaxation time strongly depends on the porous structure with varying pore size distributions. To quantify the dynamical heterogeneities and find the associated length scale, we compute the four-point correlation function. Interestingly, the length scale increases as the average pore size becomes smaller. This work sheds light on the intricate interplay between the topology of confinement and the dynamics in supercooled liquids, to understand their behavior in complex restrictive geometries.

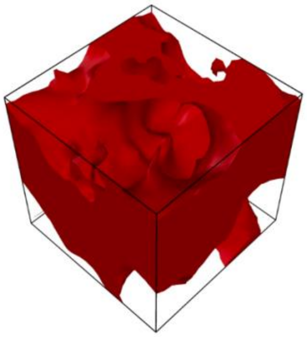

Fig. 1. Confining structure

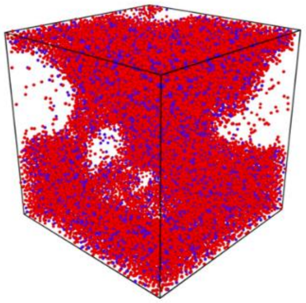

Fig. 2. Confined liquid

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Applications of κ-carrageenan hydrogels strengthened by mixed salt for 3D printing and water remediation

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Abstract

κ-carrageenan is one of the seaweed-derived polysaccharides that is commonly used in the food additive and pharmaceutical industry. In one work, we studied the gelation of 0.25-2 % w/v κ-carrageenan with potassium chloride, calcium chloride, and mixed salts by rheology, FTIR, and SEM. A synergistic increase in storage modulus was obtained with the mixed salt of KCl and $CaCl_2$.

We then assessed the printability of these hydrogel inks based on a simple extrusion process. The two extrudable pregel inks were further characterized using rheological measurements to mimic the printing process. The 3D printing of the two optimized inks was conducted using an Allvei 3 3D printer.

The printing parameters were optimized to obtain maximum pore printability of the hydrogel scaffolds. A simple model was used to predict the filament width and was compared to the printed scaffolds. Live/dead assay for human lung cancer cells seeded on the printed scaffolds was conducted, and cell viability > 95 % was observed.

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In another work κ-carrageenan hydrogel beads containing TiO_2 nanoparticles were prepared by a simple injection technique, the beads were then crosslinked in a mixed salt solution of KCl and $CaCl_2$ to increase their strength.

The rheological analysis of hydrogel discs prepared in a similar manner was conducted to approximate the elastic properties of the beads. It was observed that the crosslinking of discs using mixed salt led to a synergistic increase in modulus. κ-carrageenan/TiO_2 beads crosslinked by mixed salt had higher storage modulus, higher adsorption capacity, and stability as compared to beads crosslinked by single salt.

The κ-carrageenan/TiO_2 beads were tested by systemic study for the adsorption of 10 to 500 ppm Methylene Blue. The beads were also tested for the adsorption and degradation of multicomponent dye systems. The κ-carrageenan/TiO_2 beads could degrade up to 78% of 5 ppm Methylene Blue in 210 minutes. These biopolymer beads could be regenerated by UV irradiation and reused. The beads were further tested as column packing in a syringe for the adsorption of single and multicomponent dye systems.

Keywords: κ-carrageenan; hydrogels; rheology; 3D printing, dye degradation.

Transport properties of a fluid interacting via Mie Potential

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In the current work, we examine a two-dimensional system of particles that interact through a Mie(*2n,n*) potential, focusing on its transport properties[1]. By varying the exponent *n*, we manipulate the repulsive and attractive components of the potential, thereby influencing the interaction range. Our approach involves subjecting the system to a canonical ensemble in a high-temperature liquid state, followed by a rapid temperature quench using molecular dynamics simulation[2]. We calculate both the mean-square displacement (MSD) and the self-intermediate scattering function (Self-ISF) in proximity to the liquid-solid transition temperatures[3]. Our analysis delves into the impact of interparticle interaction range on MSD and Self-ISF. Furthermore, we determine the self-diffusion coefficient and relaxation time from the MSD and Self-ISF data, respectively, and examine their interrelationship. Additionally, we investigate the temperature dependence of the transport properties for a given system. To deepen our understanding, we calculate the activation energies associated with distinct interaction potentials by exploring the Arrhenius behavior of the self-diffusion coefficient in the high-temperature liquid state[4].

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Characteristics and correlations of nonaffine particle displacements in the plastic deformation of athermal amorphous materials

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When an amorphous solid is deformed homogeneously, it exhibits heterogeneous plastic instabilities with a localized cooperative rearrangement of a cluster of particles in response. The heterogeneous behavior plays an important role in deciding the mechanical properties of amorphous solids. We employ computer simulations to study the characteristics and the spatial correlations of these clusters characterized by their non-affine displacements in amorphous solids under simple shear deformation in the athermal-quasistatic limit. The clusters with large displacements are found to be homogeneously distributed in space in the elastic regime, followed by a localization within a system-spanning shear band after yielding. The distributions of the displacement field exhibit a power-law nature in the elastic regime with an exponential cutoff post yielding. The non-affine displacements show strong spatial correlations, which become long-ranged with increasing strain. From our results, it is evident that the decay of the correlation functions is exponential in nature in the elastic regime. The yielding transition is marked by an abrupt change in the decay after which it is well described by a power-law with an exponential cutoff. These results demonstrate a scale-free character of non-affine correlations in the steady flow regime. These results are found to be robust and independent of the strain window over which the total non-affine displacement is calculated.

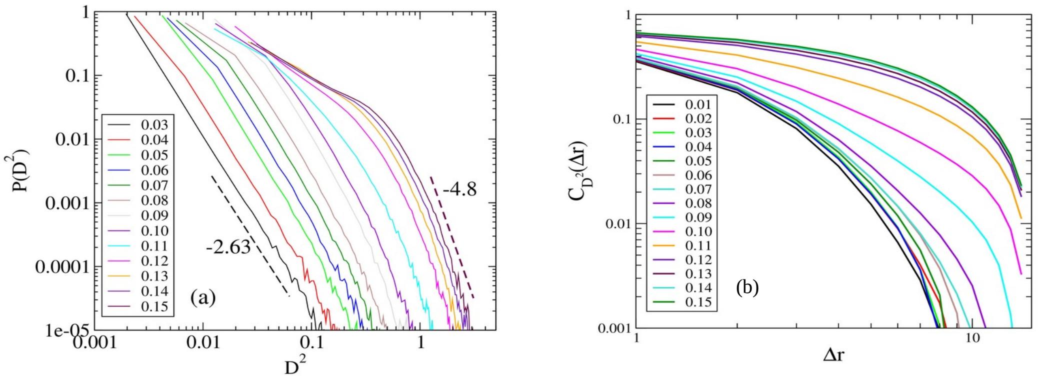

Figure 1: The distribution and the correlation of the non-affine displacement field associated with plastic deformations in amorphous solid are shown in (a) and (b) respectively.

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Effects of Salt Concentration on EC-LiTFSI Electrolytes

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Abstract:

Concentrated electrolytes have the potential to improve the stability of batteries. In this work, we studied the ion transport mechanism and ionic conductivity in highly concentrated EC-LiTFSI electrolytes, as well as its relation to ionic conductivity. Using molecular dynamics simulations, we generate long trajectories (~250 ns) of the electrolyte systems at varying salt concentrations ranging between 0.005 M and 2.5 M. Ionic conductivity increased at low salt concentrations before declining at salt concentrations above 0.7 M. We demonstrate that the salt-induced changes in ion-ion correlations and the formation of ion aggregation are intrinsically related to Nernst-Einstein and so-called *true* ionic conductivity. Additionally, we found that the viscosity is absolutely connected to the ion-pair relaxation timescales of EC-LiTFSI electrolytes as $\tau_c \sim \eta^{1.2}$. We have also found that the diffusion coefficient is connected to the viscosity and ion-pair relaxation timescales of EC-LiTFSI electrolytes as $D_{\pm} \sim \eta^{1.4}$ and $D_{\pm} \sim \tau_c^{1.1}$.

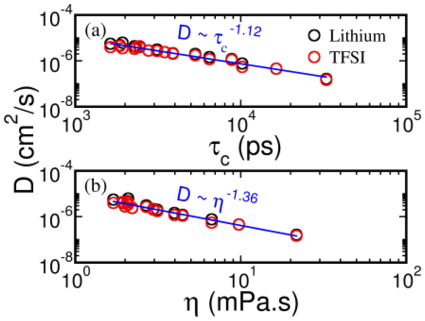

Figure 1: Diffusion coefficient compared against the ion-pair relaxation timescales (top panel) and the viscosity (bottom panel)

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Indian Society of Rheology

Ion Transport Mechanisms in PEO-SN-LiTFSI Electrolytes

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We used atomistic molecular dynamics simulations to investigate the impact of the succinonitrile on the transport properties and underlying transport mechanisms of ions in PEO-LiTFSI electrolytes. We also investigated the effect of temperature on the transport and structural properties of the electrolytes. It has been observed that the diffusivity of the ion increases as the SN loading increases, which can potentially enhance the ion conductivity of the system. By examining the transport mechanisms in SN-loaded systems, we observed that the diffusivity of TFSI ion correlates excellently with structural relaxation. Interestingly, the diffusivity of Li-ion uniquely does not depend on the ion-pair relaxation timescales but additionally depends on the polymer dynamics. Overall, our simulation results suggest that the cation-anion interactions and the polymer segmental changes influence the diffusivity of ions upon the addition of SN into the PEO electrolytes.

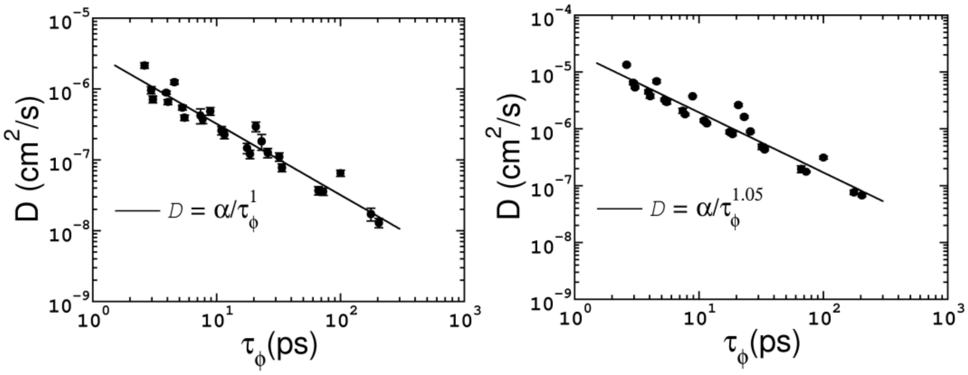

Figure 1: Diffusivity as a function of dihedral angle relaxation time for Li (left) and TFSI ions (right).

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Molecular dynamics simulations of the effect of fluorinated ethylene carbonate on sodium ion battery electrolytes

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Sodium-ion rechargeable battery electrolytes have recently gained significant attention over their more popular lithium-ion counterparts due to their abundance and safety. In this work, we use atomistic molecular dynamics simulations to study the structure and ion transport characteristics of PEO-NaPF$_6$ electrolytes and examine their dependency on fluorinated ethylene carbonate (FEC). Our simulations reveal that the diffusion coefficient of PF$_6^-$ is higher than that of the Na$^+$ ions due to weaker interactions of PF$_6^-$ with polymer. Further, the ion diffusion is found to increase monotonically with the loading of FEC. The increase in diffusion is observed to arise because of the FEC-induced faster ion-ion relaxations in the electrolyte. Our analysis reveals that sodium ions exhibit interesting ion hopping analogies to the extensively studied lithium-ion hopping along PEO backbone. The study extends its analysis to elucidate the interplay of FEC in influencing the formation of solid electrolyte interphase and the transport properties.

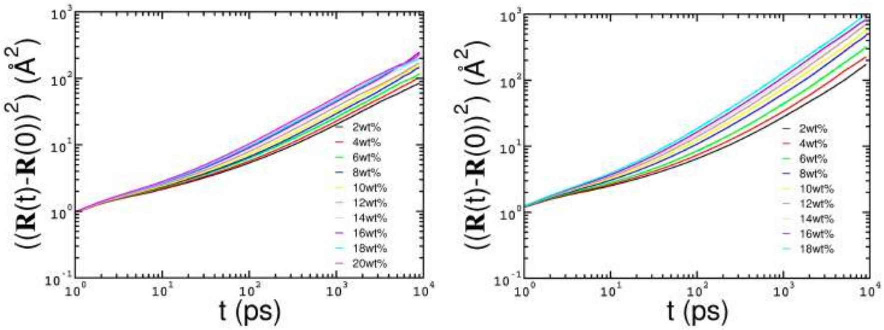

Figure 1: Mean squared displacement of sodium and PF$_6$ ions in PEO-FEC-NaPF$_6$ electrolytes.

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New Approach to Prepare FmKP based Supramolecular Organo-Gels

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The low molecular mass organo-gels (LMOG) are soft materials which embraces more attention due to its wide applications in various fields. Although numerous low molecular weight (LMW) gelators, which gelate organic solvents, have been developed in the past, but very limited reports made on solvent and oil based supramolecular gels. In this context we prepared supramolecular organo gel using Fluorenylmethoxycarbonyl-Lys-(Pal) OH (FmKP) gelator in organic solvent and base oil. Organogels have been thoroughly characterized using various spectroscopic techniques. The results of fourier transform infrared spectroscopy (FT-IR) and fluorescence spectroscopy confirm that the formation of entangled nanofibrillar morphology with ordered self-assembly of gelators, which stabilises by aromatic π–π interactions of fluorenyl moieties and hydrogen bonding interactions between –CO–NH– groups. Further, the organo gel shows thermo-reversible properties and mechanical strength which is more advantage in lubricating performance.

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Steady and oscillatory states in the granular flow through a vertical channel

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The flow of a granular material under gravity between two vertical walls separated by a width 2W is simulated using the discrete element method (DEM) using the configuration shown in figure 1. Periodic boundary conditions are applied in the flow (vertical) and the other horizontal directions. The mass flow rate is controlled by specifying the average solids fraction $\bar{\varphi}$, the ratio of the volume of the particles to the volume of the channel. A steady and fully developed state can be achieved for a narrow range of volume fraction, $\bar{\varphi}_{max} > \bar{\varphi} > \bar{\varphi}_{cr}$, and the material is in free fall for $\bar{\varphi} < \bar{\varphi}_{min}$. For an intermediate range of volume fractions ($\bar{\varphi}_{cr} > \bar{\varphi} > \bar{\varphi}_{min}$), there are oscillations in the horizontal coordinate of the centre of mass, the velocity components and the stress. The amplitude of the oscillations increases proportional to $\bar{\varphi}_{cr} - \bar{\varphi}$, and the frequency tends to a finite value, indicating a super-critical Hopf bifurcation. The relation between the fundamental frequency and the higher harmonics of the position, velocity and stress fluctuations are explained using momentum balance. It is found that dissipation in inter-particle and particle-wall contacts is critical for the presence of an oscillatory state—if the friction coefficient or the wall damping coefficient is set equal to zero, there is no oscillatory state, and there is a transition from a steady flow to an accelerating flow as the volume fraction decreases.

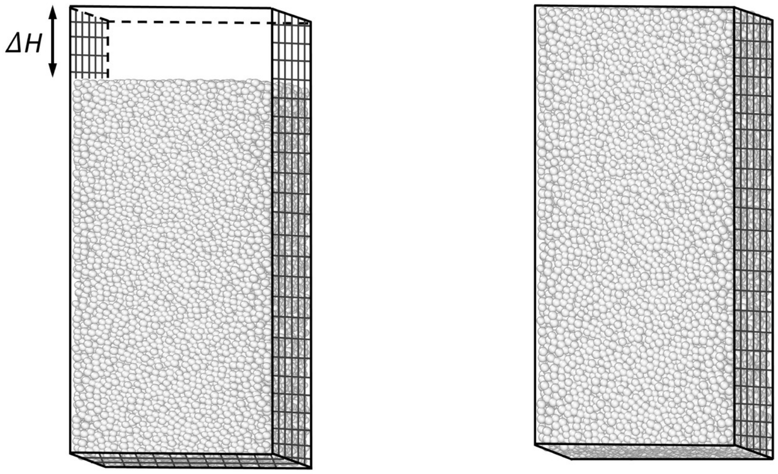

Figure 1: The initial (left) and flowing (states) of a granular material in a vertical channel.

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Spherical tracer induced clogging behavior of aspherical particles in a silo

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The clogging of the exit orifice of a silo during the outflow of granular materials is a ubiquitous problem which occurs due to formation of stable arches of flowing granular particles in the vicinity of exit orifice. The clogging phenomena has studied widely with different strategies suggested to reduce the occurrence of clogging, viz. obstacle near exit, multiple orifices and vibration or jetting. In the current work we study the effect of tracer particles with different sizes and volume fractions (ranging from 0 to 0.1), on the clogging behavior of highly aspherical particles (cylindrical shaped particles with elliptical cross-section) by performing experiments in quasi-2D rectangular flat bottomed silo. The mean avalanche size (material collected during the outflow till the occurrence of clogging) shows a non-monotonic dependence on the tracer particle concentration as well as size. For a fixed tracer particle size the clogging phenomena enhances at small concentrations while it progressively decreases at high concentrations. On the other hand for a fixed tracer particle concentration, the clogging phenomena enhances at very small as well as very large particles sizes. While decrease in the clogging tendency at higher tracer concentrations is expected given the increasing presence of smaller tracer particles compared to the orifice width, the behavior at small concentrations is quite non-intuitive. In a similar vein, the enhancement of clogging at larger tracer particle size is expected given the disappearance of its tracer identity, but the enhancement at very small particle sizes is non-intuitive. To understand the observed perplexing and non-intuitive behavior, we have performed discrete element method (DEM) simulations using LIGGGHTS. The cylindrical shape bulk particles with an elliptical cross-section are modelled using multisphere method to reasonably approximate the aspherical shape. Based on the simulation results, we are able to explain the observed behavior based on the role of particle kinetic energy and packing fraction in the vicinity of the arch formation.

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A numerical study for multi-layer powder spreading in metal additive manufacturing

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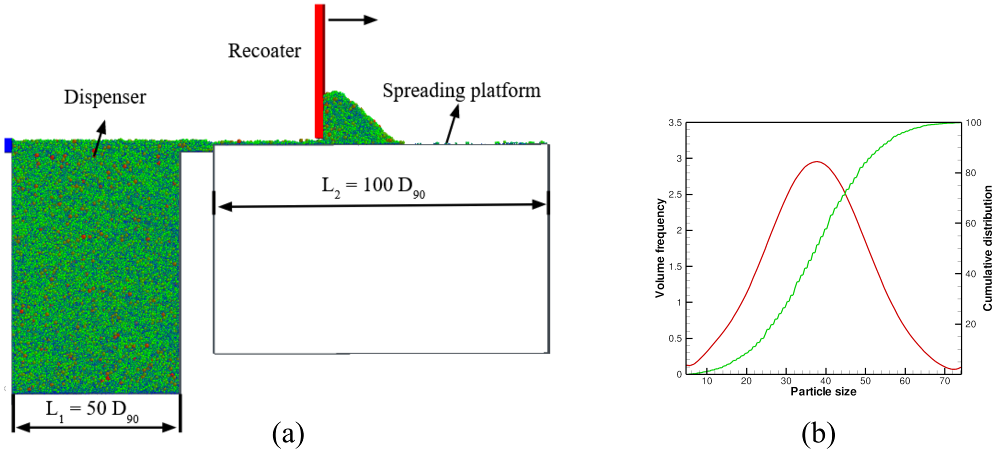
ABSTRACT

Powder bed fusion (PBF) is a metal additive manufacturing technique that uses metallic powders to produce components with high dimensional accuracy. The PBF comprises two steps - powder spreading and powder fusion. Powder spreading is the fundamental and most important process, as the homogeneity of the powder bed produced by spreading determines the quality of the final parts. The experimental investigations revealed variation in the particle size distributions at the extreme ends of the spreading zone, indicating segregation within the powder bed[1]. Several previous studies have numerically examined the segregation of powders during the spreading process. However, studies were limited to single-layer spreading simulations. In the present work, Discrete Element Method (DEM) simulations were carried out to analyse the multi-layer spreading process, as shown in Fig. 1. The packing fraction of the spread layer initially increases during the spreading process and then reaches a constant value. The simulation results also revealed the variation in the packing fraction and particle size distribution on different zones of the spreading platform. This work optimises process parameters to improve bed quality and contributes to a better understanding of the powder spreading process.



(a) (b)

Figure 1: (a) Simulation setup of powder spreading process. (b) Particle size distribution of powders used in the simulations.

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Determination of rotational coefficient of restitution from DEM simulation of vibro-fluidized particles

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In the hard-sphere collision model, particle advancement is based on the pre and post collisional velocities. Many authors have reported that various post-collisional parameters can be directly related to the pre-collision parameters[1,2]. Using a hard-sphere model, the effect of the angle of impact and friction coefficient over contact behavior is discussed [3]. However, most of these understandings are developed for two particle simulation. To the best of our knowledge, no one has reported the applicability of such analysis in a multi-particle system.

To achieve that goal, a soft-sphere modelling approach is used for the simulation of 6400 inelastic and rough particles in a vibro-fluidized bed. Contact force is modelled using linear spring and viscous dashpot. Normal stiffness (k_n) of $2 \times 10^8\, mg/d$ is used to simulate particles in the hard-sphere limit [4]. Simulations are performed for different ratios of tangential to normal stiffness, $\left(\frac{k_t}{k_n}\right)$ of 2/7 and 3/4. Individual particles are tracked to obtain their pre and post-collisional slip velocities to determine the rotational coefficient of restitution (β) and its dependence on tangential spring stiffness.

β is plotted against $\frac{7}{2}\left(1 + e_n\right)\frac{v_n}{v_s}$ in fig. 1 [3]. In case of k_t/k_n of $\frac{2}{7}$ simulation results shows two regimes i.e. sliding regime represented by positive slope regime of β profile and sticking regime represented by the the numerical values of β very close to 1 and independent of the scaling. In case of k_t/k_n of $\frac{3}{4}$, three different regimes i.e. sticking, sticking-sliding and gross sliding regimes are observed [1].

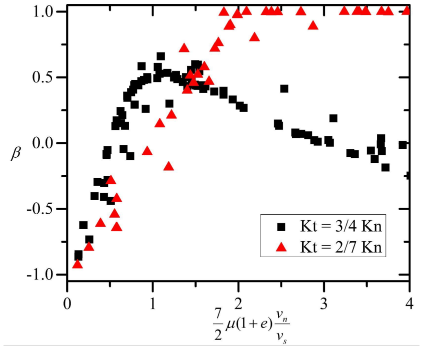

Fig. 1: β plotted against $\frac{7}{2}\left(1 + e_n\right)\frac{v_s}{v_n}$ for different ratios [2].

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Numerical investigation of the response of granular matter under high-speed impact

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Technical presentation

In this work, we employed large scale numerical simulations to understand the response of the granular media under a high speed impact. Although the large volume of the work on granular impact exists in the literature, but most of the approaches to tackle such complex problem is heuristic with no grain scale understanding of the highly dynamic impact phenomenon. This work presents the detailed microscopic length scale picture of the impact process in terms of the evolution of the inhomogeneous force chain networks, full displacement field and the velocity field as the impact progresses. These particle scale informations proved to be quite useful in understanding the dissipation mechanism in the granular materials which is neither solid nor fluid. One of the key findings of the work is the discovery of a novel energy dissipation mechanism in granular media through the propagation of acoustic pulses which reach the end of the system boundary even though the system size is large enough to avoid boundary effects. This very fast large length scale propagation of disturbances is evocative of the collective motion of the granular particles which are correlated upto long range even before the impact. We also observe reflection of the acoustic pulses from the boundary as well as sideways scattering and branching of the pulses. Reflected pulses also interacts with the original pulses emitted from the intruder and gives rise to destructive interference. The wild fluctuations in the force time series of the intruder is attributed to the constant large scale reorganization of the force chain networks. The strength of the fluctuations vary with different system parameters like intruder mass, diameter, bed properties like packing fraction, friction coefficient etc. We also observe some critical phenomena with respect to the force response and correspondingly the velocity time series when the initial impact velocity and the intruder diameter reaches some threshold value. We also extensively studied the effect of different pertinent parameters on the penetration depth and forces exerted by the granular media on the intruder. Lot of our scaling relations are completely new and some of them also contradict the existing literature as most of the experimental works did not capture the fast time scale dynamics due to the technological restrictions. The finding of this research will find immediate application in the space industries, ballistics and any other process involving high speed impact. In Fig 1., we show the evolution of the force chain network as the impact progresses. Fig 2. shows the time evolution of the force on the intruder.

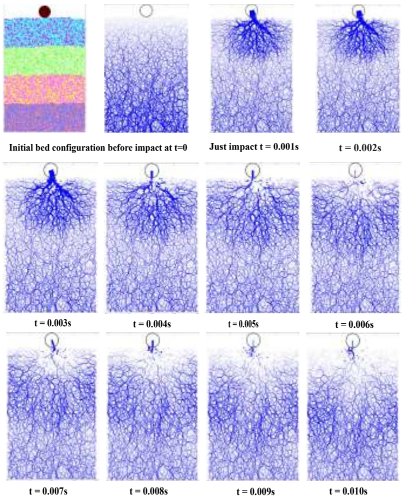

Figure 1: Force chain networks at different stages of impact

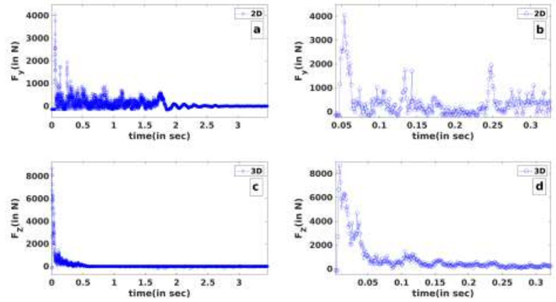

Figure 2: (a)Force on the intruder in y direction(gravity is acting in -y direction) (b)Force on the intruder in the initial stages in 2D. (c)Force on the intruder in z direction(gravity is acting in -z direction) (d)Force on the intruder in the initial stages in 3D

Mechanical behaviour of cohesive frictional granular materials

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and
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Granular materials consist of discrete solid particles which interact with each other via interparticle contact friction. In the presence of small amounts of cohesive forces between the particles, the mechanical response changes dramatically. We report two sets of experiments where we examine the effect of cohesive binder on the kinetic and kinematic behavior of frictional granular materials.
We carefully parse the kinematics during deformation of a cohesive granular ensemble, using a combination of x-ray computed microtomography at high resolution. Under a range of boundary conditions, we report on how the interparticle cohesion breaks down at reasonably small strain levels, following which frictional interaction ensues. We examine the progressive changes in the cohesive binder network across micro and meso-length scales as loading progresses. In addition, we resolve the kinematics for various degrees of cohesion and model granular ensembles.

We complement these experiments with 2D photo-elastic discs to replicate a cohesive granular ensemble. We study these systems under different traction boundary conditions (Pure shear, Uniaxial compression, Isotropic compression), and quantify the changes in force propagation in these systems with and without cohesion. It is well known that surface tractions are resisted by the formation of chain-like structures. These chains are highly heterogeneous and span the entire granular structure. In our experiment, we solve the inverse problem to obtain force magnitude and direction at each particle-particle contact . Force distribution for uniaxially compressed ensemble shows an exponential dip for higher loads (greater than the mean force), while the contacts are roughly oriented along the major principal normal stress direction.

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Role of elasticity and cohesion for accurate and efficient simulations of cohesive granular materials

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Cohesive granular materials are a common occurrence in many industrial settings. Different cohesive force models are used in DEM simulations to account for the effect of cohesion between particles. However, simulation parameters used in different cohesive force models are often chosen in an adhoc fashion. The particle sizes, cohesion and elasticity parameters used in the literature vary over three to four orders of magnitude. In this study, we compare three different cohesion models commonly used in open-source and commercial DEM simulation software. In order to establish a connection between cohesive parameters of two different models, detailed theoretical analysis of the equation of motion of a cohesive particle interacting with a wall is undertaken. The equation is non-dimensionalized to determine the relevant dimensionless numbers for each cohesion model. DEM simulations of a cohesive single particle interacting with a flat wall are performed to confirm our theoretical predictions. Using these appropriate non-dimensional parameters, we obtain a phase space relating the particle deformation to the cohesion parameter and the elastic parameter of the model and identify appropriate limits for these parameters for accurate and efficient simulations. Simulation studies used in the literature are then mapped to this phase space to identify the appropriateness of the parameters selected elasticity and cohesion. In order to explore the applicability of our findings to a multiparticle system, we perform DEM simulations of cohesive frictional, spherical particles filled in a container of rectangular cross-section under the influence of gravity. The results obtained give insight into the important effects that need to be considered during the simulation of cohesive grains.

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Self-organization of granular systems under chiral driving

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We study a monolayer of metal balls under periodic chiral driving in the horizontal plane. Energy dissipation occurs in this system via (i) inelastic inter-ball collisions and (ii) ball-substrate interaction characterized by the coefficient of friction. Since balls can both roll and slide, the system has access to varying coefficients of friction depending on the fraction of time balls spend in rolling and sliding states. The transition between rolling and sliding is brought about by inter-ball interactions. We show that the present system phase separates into a mobile (liquid like) and an immobile (clustered) phase below a critical driving frequency. We also find that the average mechanical force in the system changes discontinuously over the critical driving frequency.

Flow kinematics and stress comparison of resolved and multi-level coarse-grained DEM simulations

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The Discrete Element Method (DEM) has proven to be a robust computational tool for simulating bulk solids in diverse engineering systems. Industrial-scale simulations of bulk solids using DEM involve an enormous number of particles, making coarse-graining an effective technique to alleviate computational demands. In coarse-graining, a group of resolved particles are replaced with coarser particles with the necessary changes in the particle properties to mimic the resolved simulation. Thus, the overall number of particles reduces which leads to lesser computational cost. However, conventional coarse-graining methods often employ uniform coarse-grain ratios throughout the equipment, limiting the degree of coarse-graining due to potential accuracy issues at higher ratios. To address this challenge, a novel multi-level coarse-graining technique (MCG) has been recently proposed by De te al. [1], offering variable coarse-grain ratios throughout the geometry. In this research, we delve deep into the flow kinematics and stress analysis aspects of the MCG technique, showcasing its practical applicability in solving engineering challenges. We explore various scaling laws for contact forces and propose appropriate scaling laws for both the linear spring dashpot model and the Hertz-Mindlin model for the MCG technique. Our findings demonstrate the effectiveness of the MCG approach in significantly reducing computational costs while retaining essential details of flow and stress fields in large-scale industrial simulations. By presenting the improved scaling laws for contact forces, this study opens avenues for more accurate and efficient simulations of granular materials in various engineering applications.

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Indian Society of Rheology

Influence of rheology on the pipeline transportation of mineral slurries

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Conveying mineral slurries through the pipeline offers many advantages, including minimum environmental disruption, less en-route losses and pollution, feasibility in adverse locations, and surface conditions [1]. One of the major concerns related to slurry flow is obtaining favourable flow behavior in the pipeline. Here, the rheological studies play an important role in describing the flow characteristic of the slurry in the pipeline.

The primary focus of the present study is to demonstrate the role of particle concentration and size distribution on slurry rheology and its influence on slurry pipeline transportation. The rheological analysis reveals the shear thinning flow behaviour of bauxite slurries irrespective of particle concentrations and sizes. The slurry with fine particles enhances the viscosity (Figure 1(a)), which is reduced by incorporating an optimum concentration of coarse particles. Interestingly, the viscosity does not change appreciably after exceeding the critical coarse particle concentration. Rheo-microscopy studies support these rheological interpretations, suggesting that the dense floc structures of the fine slurry disintegrate with increasing coarse particle concentration and applied shear rate, resulting in reduced viscosity (Figure 1(b) and (c)). Moreover, the flow coefficients obtained using the rheological model [2] are used to estimate the pipe flow parameters. It is proposed that optimizing rheology parameters lowers the cost of pipeline transportation while handling bulk quantities of particulate solids to longer distances.

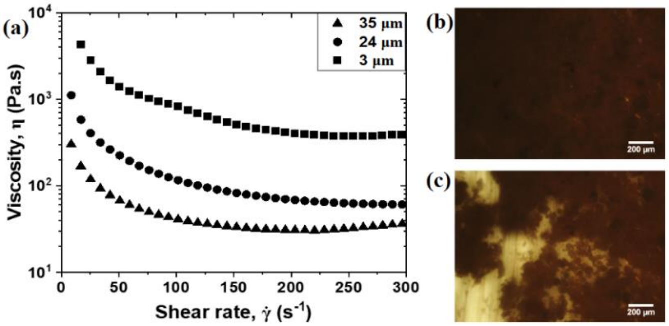

Figure 1: (a) Viscosity as a function of particle size. Rheo-microscopy images of slurries with (b) fine (d_{50} = 3 μm) and (b) coarse (d_{50} = 35 μm) bauxite particles

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Assessment of Segregation for Non-spherical Cohesive Particles using DEM

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Industrial particles are mostly nonspherical. The objective of this study is to analyze the synergetic effect of particle shape and particle cohesion on segregation behavior of binary mixtures in vibrating packed bed using discrete element method (DEM) simulation. Sphere and ellipsoid group prolate particles of sizes 6 mm and 4 mm are simulated using cohesive SJKR model. The binary mixture is mixed at constant vibration intensity which is a measure of added energy to the system. The mixing profile shows for cohesive particles the mixing is decreased as compared to non-cohesive spherical-prolate mixture due to agglomeration or clump formation. Also, the binary mixture of spherical-nonspherical gives better mixing compared to the binary mixture of spherical-spherical. Therefore, an increase in non-sphericity decreases segregation. In addition, the evolution of cohesive particles to the final mixed equilibrium state of the system depends more strongly on the initial state i.e., whether it is started as uniformly mixed or totally segregated. Results have important design implications and help provide heuristics to reduce segregation when taking both particle cohesion and non-sphericity into account.

Keywords: Non-spherical particle, Cohesion, Segregation, SJKR, DEM

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Granular Morphology Matters: Deformation Mechanics of Lithium-Based Pebbles under Triaxial Compression

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Our research proposes a framework that uses the open-source DEM (Discrete Element Method) tool LIGGGHTS[1] to conduct triaxial compression simulations of pebble beds[2] and to determine the Drucker Prager (DP) model parameters for various pebble morphologies. The primary objective of this study is to investigate the mesoscopic behaviour of monodisperse, polydisperse, and ellipsoidal pebble granular systems by conducting a series of drained triaxial compression tests. The mesoscopic response was evaluated concerning deviatoric stress and volumetric strain with respect to axial strain. The initial yield behavior of the DP plasticity model was estimated from the mesoscopic response.

In this study, a monodisperse particle system with varying packing fractions (approximately 60 %, 62 %, and 64 %), interparticle friction (0.1 to 0.9), and rolling friction (DCT[1] and EPSD[1] friction models from LIGGGHTS) was examined. A polydisperse particle system was also analyzed with varying degrees of polydispersity (pebble radii ranging from 0.1 mm to 0.9 mm). Furthermore, ellipsoidal particles with different aspect ratios (1.0, 1.25, 1.5, and 2.0) were studied. After generating data for all the granular systems, a comparative study was conducted using post-processing tools. Voronoi tessellations help to visualize the local environment during compression, enhancing the understanding of the deformation behaviour. Additionally, microstructural evolution analysis enabled the quantification of particle involvement during deformation. Furthermore, a comparative study was conducted to evaluate and compare various parameters, exploring the similarities and dissimilarities in the microstructural evolutions during triaxial compression.

keywords: Pebble bed, DEM, LIGGGHTS, Drucker-Prager model, DCT (Directional constant torque model), EPSD (Elastic-plastic spring-dashpot model).

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Flow behavior of lubricated granular media across various flow configurations

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The inter-particle interaction plays an important role in the overall flow behavior of granular materials, the friction and collision being the predominant modes of interaction. In our earlier work (Ghodake et al., *Powder Technol*. **2022**), we showed that partial coating of granular material (glass beads) by a suitable solid lubricant can improved the flowability, albeit over a narrow range of lubricant concentration, with the behavior deteriorating for very small and large lubricant concentrations. In the current work, we have explored the effect of lubricant for different materials and different geometry with a view to understand the universality of the lubrication behavior.

Experiments were performed in Couette geometry, flat bottom silo and inclined chute system for various concentrations of Magnesium Stearate as the lubricant with four different granular materials, viz. glass beads, mustard seeds, sagu beads and granulated Lactose powder. The non-monotonic dependence of the flowability on lubricant concentration was observed in all the geometries and for all the material types used. However, the concentration range corresponding to maximum flowability was found to be dependent on the flow geometry and the particle type. The effect of lubricant was observed to be the most pronounced in Couette geometry, while the flow in silo system showed minimal dependence on lubricant concentration. Further, the smoother glass beads exhibited maximum flowability over a smaller lubricant concentration range, while the improved flowability occurred over a wider range for rough surfaced Lactose granules. Most interestingly, the maximum flowability seems to occur over the same lubricant concentration range for a given particle type. The overall behavior can be explained qualitatively by microscopic imaging of lubricant coated particle surfaces.

Reference: Ravindra S. Ghodake, Pankaj Doshi, Ashish V. Orpe, *Powder Technol.*, **409**, 117809 (2022)

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Flow characterization of poly-dispersed granules under the influence of external mechanical vibration for additive manufacturing applications

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The quality of a product fabricated using a granular-based process depends on the flow characteristic of the feed-stock particles. Controlled flow is essential for the homogeneous distribution of the granules. For poly-disperse granules considering cohesion between the particles, segregation and agglomeration is a major challenge for arching phenomenon for particle size range from 40 μm – 200 μm [1]. One way to enhance this control is by using vibration-assisted flow [2]. Although dry particulate flows in vibration hoppers are a popular area to researchers but the information extracted was limited and deficient to show the mechanism behind the dynamics of the particles. A hopper model of 2 mm internal exit diameter with sinusoidal excitation in horizontal direction was developed as shown in figure 1. The influence of external mechanical vibration on the granular flow is investigated using discrete element simulations. The work also reports the influence of cohesion between particles, vibration intensity, hopper and particle ratio on the flow characteristics. The research facilitates the effective use of mechanical vibration to enhance granular flow that can further be extended to non-spherical and multi-material particles.

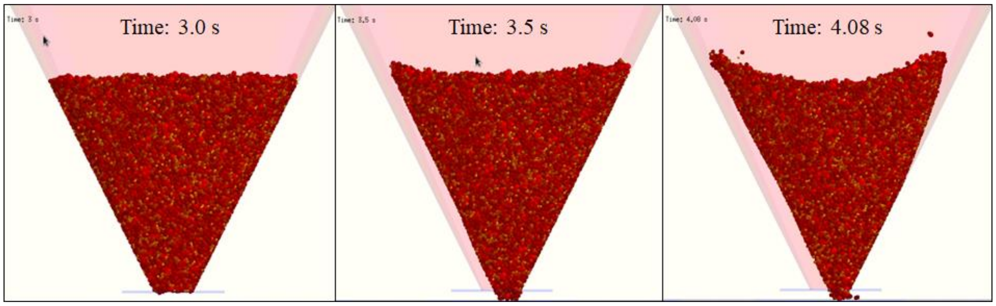

Figure 1: Gravity-driven granular flow of poly-disperse particles (40 – 160 μm) under influence of horizontal vibration.

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Indian Society of Rheology

A Computational Study on the Smooth-Wall, Radial Gravity Phenomenon in Granular Flow Through a Wedge-Shaped Hopper

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Hoppers with inclined walls are used in industry, where materials flow by gravity and exit through a bottom outlet. The simplest form of this flow can be described as a wedge-shaped, quasi-two-dimensional geometry with smooth walls, influenced by radial gravitational forces. Theoretical analysis of this flow has been conducted using the Mohr-Coulomb criterion in the classical work of Savage (1965) and using a critical state theory by Ravi Prakash and Rao (1988). To validate the existing theories, discrete element method simulations are performed on particles within a smooth-wall radial gravity wedge-shaped hopper, obtaining detailed stress and velocity fields. Our computational results match with the predictions of the existing theories, except in the region near the exit where both frictional and viscous effects are present. To further understand this behavior, we conducted a parametric study on wedge-shaped hoppers, varying parameters such as orifice size, wedge angle, friction coefficient, and stiffness. This study investigates the influence of frictional walls and vertical gravitational forces on the system's behavior, aiming for a comprehensive understanding. The transient outcomes are compared to the average behavior to deepen our understanding, and the results are presented. And also, empirical correlations quantify the relationships between stresses at the exit, considering frictional and viscous forces. In particular, the correlation between viscosity and shear rate at the exit is important, as it captures the effects of momentum and particle transfer during collisions, exhibiting a significant dependence on viscosity near the exit region. Additionally, it is demonstrated that viscosity and volume fraction exhibit power law correlations with the inertial number proposed by Jop et al. (2006) and that all the data collapse into a single curve, enhancing our understanding of granular material behavior for such flow prediction.

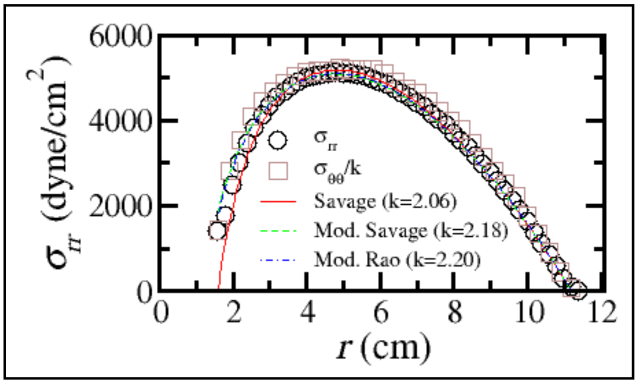

Figure 1: Stress in *r-direction* as a function of radial diatance.

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Two-phase approach for laminar shearing beds using kinetic theory of granular flows

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Fluid-solid flows have a variety of applications both in industries and environmentally, to name a few, fluidized bed jet mills, bedload and suspended load transfers. Over the past few decades, due to the development of satisfactory experimental and computational approaches, the understanding of granular flows have evolved significantly. Shearing flows leading to erosion of granular beds despite the fact of importance, the thorough understanding has been lacking. Most of these applications and also existing literature concerns about turbulent regimes but it is to be noted that laminar flows also generate similar patterns subjected to a critical shields number (independent of Re). Based on Shields number, the Sediment transport regimes are distinguished as bedload or suspended load.

Using two-phase Eulerian- Eulerian framework, the sediment transport regimes can be modelled and when restricted to laminar regime, the challenges lies in closure models for particle-particle interactions. Two approaches have been accessible in literature, one $\mu(I)$ rheology which is based on dimensional analysis and other is Kinetic theory of Granular flows which is been used smooth, frictionless spheresfrom decades for modelling two-phase models. Both these models have their own assumptions and imitations, $\mu(I)$ valid in dense regimes and kinetic theory in dilute. In broader sense, for an ordinary sediment bed, this separation of regions into dense and dilute regimes adds complexations and also unavailability of a single closure model to describe entire bed length has served motivation for this work. Laminar shearing beds in viscous regimes have been typically solved either using $\mu(I)$ rheology or by combining Coulomb's friction with Einstein viscosity. The proposed work focusses on using a two-phase model incorporated with kinetic theory closure for intergranular stresses in viscous regime for laminar shear beds. The results are compared with existing literature using alternative closure models. The failure of classical kinetic theory closure for proposed work are disussed and modifications are proposed. The results are compared with existing literature using alternative closure models.

Key words: kinetic theory of granular flows, laminar shearing beds, sediment transport

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Kinematics of Granular Surface Flow on a Heap

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This study reports experimental results for the surface flow of nearly monodisperse, spherical stainless steel particles on a granular heap, formed by pouring stainless steel particles from a hopper through thin rectangular slits of varying widths, on to a rough base on a rectangular platform. In the central portion of the heap, the flow is unidirectional. Previous studies of unidirectional flows on an erodible heap have been carried out in channels with side walls, which have a significant effect on the flow [1,2]. The geometry is an example of surface flow on an erodible bed without any side walls. A steady, fully developed surface flow is established when the base of the heap reaches the edge of the platform. The streamwise and transverse velocities are measured using high speed videography and Particle Tracking Velocimetry.

Purely one dimensional flow of granular materials is observed in a region in the central zone on the surface of the heap. The surface velocity is nearly constant in the streamwise direction. The magnitude of the surface velocity increases with increasing mass flow rates. The surface angles measured at the flowing zone remain almost constant over a five fold increase in mass flow rates. This was also observed in a previous study for surface flow over axisymmetric conical heaps as well [3]. The flowing layer thickness was measured by immersing a coated blade into the plug flow zone and compared to a model developed using the measured surface velocities. The predicted values of flowing layer depth match the measured values reasonably well.

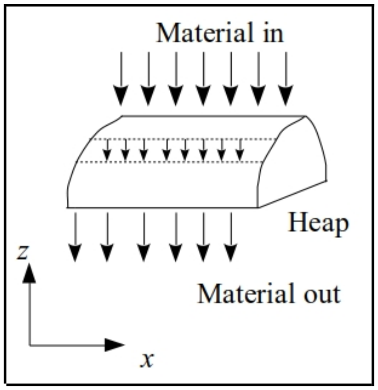

Figure 1: A schematic representation of the steady flow of granular materials in the central zone on the surface of a heap

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Large Scale Industrial Hopper Flow Simulation using coarse-grained DEM

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Large-scale industrial hopper typically contains tens of millions of particles. For example, a typical granular feed used in the blast furnace of steel industries has more than 50 million particles. Since conducting a resolved simulation proves unfeasible due to the large particle count, we employ the coarse-graining (CG) technique to better analyze the discharge rate and flow kinematics of iron ore (pellets and sinters) flowing from an industrial-size hopper. In the CG-DEM, a group of resolved particles is replaced with coarser particles with some necessary changes in the particle properties. This ensures that a larger system can be simulated with a relatively smaller number of particles. In this study, we investigate the impact of the coarse-grained ratio on the accuracy of the Discrete Element Method (DEM) simulations, specifically examining the effect on discharge rate and other kinematic properties of metallics for hopper discharge simulation. Three different CG ratios (i.e., the ratio of the radius of CG and resolved particle) have been considered in our test cases and results have been compared with the experimental measurement at TATA Steel. We find that a CG ratio of up to 3 can closely approximate the discharge rate from the blast furnace hopper employed at TATA Steel. The similarities and differences in the velocity field, packing fraction, as well as composition of the pellets and sinters are investigated in detail for different CG ratios. This study provides insights about the maximum CG ratio for accurate and efficient DEM simulations that can be utilized for large-scale industrial systems.

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Theory for combined effect of size and density segregation of binary granular mixtures

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Granular mixtures, consisting of particles that typically exhibit a large variation in size, density, shape, and surface properties, often segregate during their flow and transportation. Such particle segregation occurs readily in industrial applications and hazardous geophysical flows such as landslides. Undesired segregation also leads to a reduction in product quality in various industries such as pharmaceutical manufacturing, polymer processing, iron, and steel plants etc. In this work, we investigate the segregation of binary granular mixtures flowing over an inclined surface computationally using distinct element method (DEM) simulations and theory. DEM simulations are performed over a wide range of density ratios ($1.0 \leq \rho \leq 4.0$), and different size ratios ($r = 1.0, 1.25, 1.5, 1.75, 2.0$). A wide range of compositions of large species ($12.5\% \leq f_L \leq 87.5\%$) are considered over different inclination angles. We develop a segregation model based on particle-level forces and account for the combined effect of species size difference and density difference on the extent of the segregation. Concentration profiles are predicted by incorporating this segregation model into the continuum approach of solving convection-diffusion transport equation along with the momentum balance equations. The segregation model reduces to the earlier proposed density [1] and size segregation [2] models based on the particle force-based theory. In addition, the intercoupling of the segregation model with the rheological model is also accounted. The proposed theory captures segregation phenomena very well for the mixtures where the effect of density difference and size difference cooperate with each other and give rise to enhanced segregation. In the case of competing effects of density and size on the segregation, however, the theory is only partially successful.

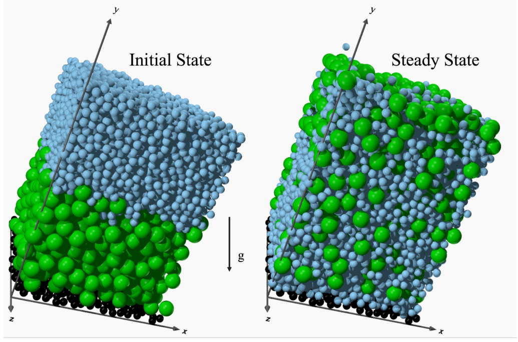

Figure 1: DEM simulation snapshot for an equal composition binary granular mixture having density ratio $\rho = 2.0$ and size ratio $r = 2.0$ flowing over an inclined plane. Green and blue particles represent the high and low density particles, respectively. Black particles represent the rough bumpy base.

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Continuum modeling of granular flow evolution using OpenFOAM

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Granular materials are commonly involved in geophysical flows and are widely used in many industries such as iron and steel, pharmaceuticals, cement, etc. The granular flow behavior is widely studied using Discrete Element Method (DEM) simulations where equations of all the particles are integrated to obtain their positions and velocities at every step. Due to the high computational cost of DEM simulations, continuum simulation of granular materials seem a more efficient option. In this work, we perform continuum simulations of 2D granular flow over an inclined chute. We extend the *multiphaseEulerFoam* solver used for two-phase fluid simulations in open source CFD software OpenFOAM for subaerial granular flow. The numerical framework involves solving the continuity equation and momentum balance equations for both the phases i.e., the fluid phase (air) and the granular phase. The granular phase is modeled as a continuum employing the $\mu(I)$ rheology while the fluid phase is simulated as a Newtonian fluid in the laminar regime. We predict the time dependent as well as steady state flow properties such as velocity, pressure, and shear stress using the continuum model and compare it with the DEM simulation results for a periodic chute.

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Turbulence modification of particle-laden flow in horizontal rectangular duct

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Pneumatic conveying is used to transport solids in many chemical and pharmaceutical industries. Despite its high industrial relevance, the different types of interactions, like the particle–turbulence, particle-particle, and particle–wall [1] for wall-bounded flows, are not well understood. The objective of the present work is to understand the two-phase dynamics of the particle-laden flow in a horizontal rectangular duct. Simulations are performed using the Eulerian-Lagrangian framework considering turbulent fluid medium as the continuum, and the particles are discrete Lagrangian point particles. Although point particle approximation is used to calculate drag force on the particles, their finite size effect is considered to simulate particle-particle and particle-wall interactions. The duct used in the present investigation has a cross-section of 4:1. Two-way coupling is used with the De-Felice equation to model the drag. Dynamic one equation LES is coupled with DEM for the particle phase. Simulations are performed using both perfectly smooth and rough particles. The mean velocity profiles for the gas and particle phases, shown in Figure 1, and the second moments of the velocity fluctuations are computed. It is observed that the fluid Reynolds stress decreases with the increase in the mass loading ratio, and a turbulence collapse is observed for the mass loading ratio of 1.0 when the particle Stokes number is 82.

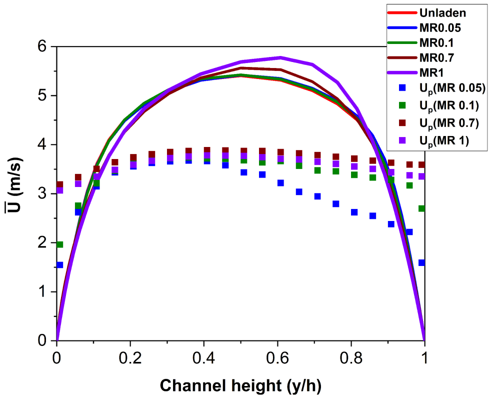

Figure 1: Mean streamwise fluid ($\overline{U}$) and particle (U_p) velocity profile for different solid to fluid mass loading ratio

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DEM analysis of inelastic rough spherical particles in a vibro-fluidised

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Vibro-fluidisation has been of interest in many applications related to transportation, handling and processing of bulk granular materials. However, the role of vibrational amplitude and frequency on the bulk behaviour of bed is still not clear [1].
In this work, inelastic and rough spherical particles in a three-dimensional vertical vibrated bed are simulated using LAMMPS. Interparticle contact is modelled using a linear spring and viscous dashpot. Simulations are first performed for perfectly smooth inealstic particles with the parameters identified in Sunthar and Kumaran [2]. Smooth case is validated with the leading-order prediction of kinetic theory (fig. 1a) as proposed in [3]. Later, simulations are extended for particles with rough surfaces. Rotational coefficient of restitution is determined based on the pre and post collisional velocities of pairs of colliding particles. It is observed that equipartition of energy exists only for nearly perfectly rough particles ($\beta \approx +1$), as suggested in Rao and Nott [4]; however, counter-intuitive to the concept of equilibrium of thermodynamic states (fig. 1b). Simulation results also show that properties like volume fraction, linear and rotational fluctuating kinetic energy determined for nearly smooth particles overlap with that of nearly perfectly rough particles. Scaling laws obtained for nearly perfectly rough and nearly perfectly smooth particles are validated with DEM results. Simulations do not show any specific trend for variation in amplitude and frequency of vibration.

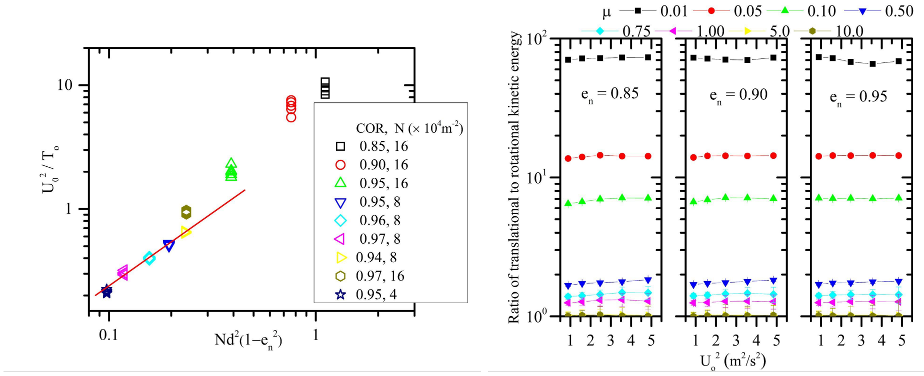

Figure 1: (a) Validation of DEM simulation for smooth particles with the prediction of kinetic theory in the limit $\frac{U_o^2}{T_o} \ll 1$. (b) Ratio of translational to rotational fluctuating kinetic energies for varying coefficient of restitution (e_n) and interparticle friction coefficient(μ).

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2D DEM study of force transmission during in-plane cutting of flexible granular chains

Keywords: Flexible granular chains, Entanglement, Interlocking, constraint, shear band.

Flexible granular chains are linear chains composed of hollow spherical beads connected together by I-shaped links (Fig. 1). Because of their flexible nature, these chains interlock and entangle, thereby providing the dry and cohesionless granular materials similar mechanical rigidity as of their cohesive counterparts. This property called “geometric cohesion" has also been observed in a variety of other interlocking particle morphologies such as U-shape, Z-shape, and rod shaped particles etc. (Gravish & Goldman, 2016). Flexible granular chains of length or number of monomers(M) greater than a certain critical chain length exhibit an array of intriguing properties such as jamming at low densities, strain stiffening and higher stiffness at smaller coordination numbers etc. (Dumont et al., 2018). Although experimental measurements have provided an insight into the kinematics of these chains at large deformation and deformation rates, the micromechanics of chain response under large deformation and deformation rates is yet to be explored.

In this study we develop and calibrate a discrete element method contact model to simulate the mechanics of the macroscopic flexible granular chains, wherein the links connecting the beads in the chains are implemented as superimposed kinematic constraints on the chain motion, with a linear normal and angular stiffness consisting a link contact (Fig. 1). The orthogonal cutting simulations are carried out with varying chain length(*M*), cutting depth (D_0), rake angle (β) and cutting speeds (v_c). We evaluate various micro-mechanical, topological and macroscopic parameters to elucidate the macro and micro-mechanical response of these chain ensembles at large deformation rates. The ability of the chains to form tensile force chains effects the formation and suppression of localised shear bands during cutting.

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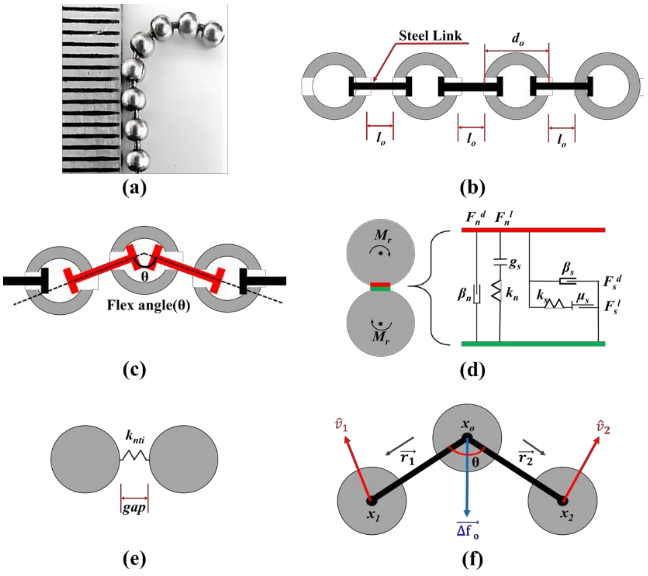

Figure 1: Geometric characteristics of the flexible granular chains (a) Photograph of the metallic flexible granular chain modelled in this study. (b) I-shaped links with a maximum elongation length of l_0 (c) Angular constraint on two consecutive links in the chain, due to their geometry (d) Contact created by the overlap of two particles shown in the red-green bar with the rolling moment acting on the contacting particles at their centres and the expanded linear contact shows the behaviour and rheological components of linear contact model implemented at frictional contacts. (e) DEM implementation of the elongation constraint in the flexible granular chain. (f) Angular constraint implementation in DEM contact model for flexible granular chains.

Dynamics of pile formation

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Granular materials are ubiquitous in nature and are handled or processed in many industries.

Despite their widespread occurrence, their behavior in static and flowing conditions is not adequately understood. It is important to understand the static stress in granular media to design devices for their storage, packaging, and transportation. However, their complex mechanical response has posed challenges in developing such an understanding. Even after decades of research, the mechanism of stress transmission in static granular media remains an open question. For static granular media, it is ~~a~~ well-established that different pouring protocols lead to different stress profiles at boundaries. In this work, we attempt to understand how microstructure rearrangement effect steady stress transmission. In particular, we try to understand source of anisotropy in granular packing. In future we will attempt to quantify the anisotropy for different geometries and deposition protocols.

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IA-O1

Saswati Pujari

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IA-O2

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Experimental investigations to study the drug release from bilayer osmotic tablets

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Controlled drug delivery systems, through the sustained release of drugs, enable the drug concentration to remain within the therapeutic range for a long time, thus increasing the effectiveness of drugs. One of the most successful delivery systemsis the oral osmotic delivery system, as the delivery of the drug is independent of external conditions such as pH and hydrodynamic conditions.

We have performed experiments on bilayer osmotic tablets in which the upper layer consists of a drug and polymer, and the lower layer consists of a swellable polymer and an osmotic agent (salt). Model (inert) particles were used instead of drug particles to understand the influence of various factors, such as orifice size and coating thickness, on the extrusion of the model drug particles. We have also designed a setup for collecting the extrudate to determine the relative ratios of polymer, osmotic agent, water, and drug in the extrudate and also to draw a comparison between these ratios and those existing in the upper layer of the tablet.To account for the reproducibility of the experiments, the experiments have been repeated twice for every time point. Next, we compared the measurements with predictions of a mathematical model that accounts for the details of the drug delivery process, namely, solvent imbibition due to osmotic pressure gradient, hydration of the drug layer, swelling of the sweller layer, build-up of hydrostatic pressure, and extrusion of the extrudate through the orifice. The results show a good agreement between measurements and model predictions, suggesting that the model captures well all the key processes involved in the drug delivery process.

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IA-O4

Role of organic ligands on the gas adsorption and separation in Zeolitic Imidazolate Frameworks

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Metal organic frameworks (MOFs) are composed of metal ions that are linked via organic ligand molecules. They are porous and crystalline in nature with high surface area. There exists a wide range of linker molecules that can tune the properties of MOFs. This makes them a promising class of material for gas separations [1]. Towards this end, Zeolitic Imidazolate Frameworks (ZIFs), which is a subclass of MOFs resembling zeolite structure as shown for a representative case of ZIF-90 in Figure 1, exhibit reversible structural transformations such as breathing, swelling, and rotation of linkers responsible for variation in volume, surface area, and pore size, etc. [2]. Here, we combine grand canonical Monte Carlo simulation (GCMC), molecular dynamics (MD) simulation and density functional theory (DFT) to develop a deeper understand of ZIFs' flexibility and its impact on gas adsorption and separation. We estimate the adsorption isotherms for CO_2, N_2, CH_4, and H_2O in several ZIFs vis GCMC simulations. We predict the diffusion of gas molecules inside the ZIFs via MD simulation. Moreover, our DFT calculations provide energetically favorable orientation of gas molecules over the adsorption site. Our work provides important design rules of ZIF materials for gas separation application.

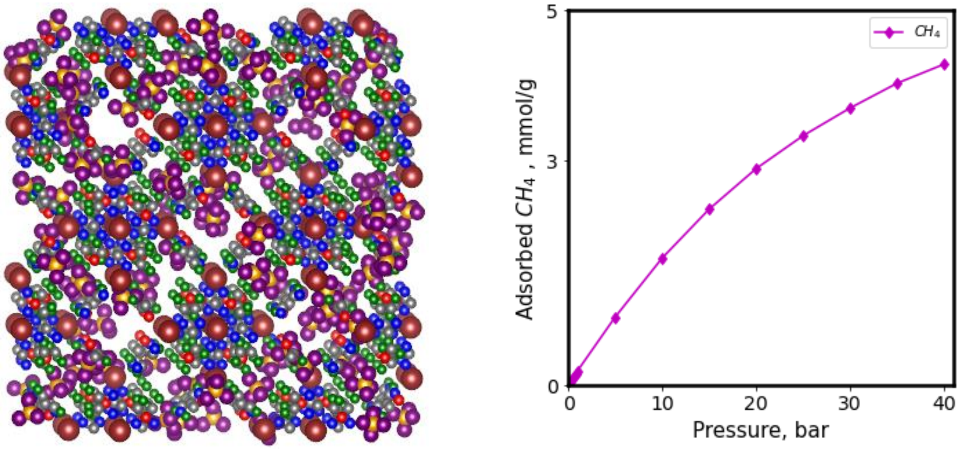

Figure 1: 2*2*2-unit cells ZIF-90, consists of zinc metal networking 2-carboxaldehyde imidazole as linkers (left), methane adsorption isotherm at 298 K (right). Carbon (grey), oxygen (red), hydrogen (green), nitrogen (blue), zinc (brown) and methane carbon (yellow), methane hydrogen (purple) are represented as spherical balls.

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IA-O5

Girish

TBD

Application of Analytical Solution of Free Radical Polymerization With AK Method For Semi-Batch Operations

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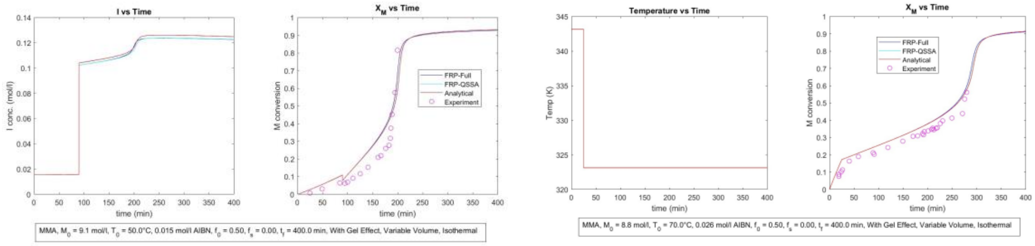
Analytical solution (AS) for free radical polymerization (FRP) with AK method for gel/glass/cage effects has been shown to give results similar to moments based complete mathematical model with 11 ODEs in our previous work [1]. The conditions for which results were compared were for fully mixed isothermal/ non-isothermal batch homogeneous solution polymerization. But it was not extended to semi-batch reactor condition which is also quite useful for controlling the polymer properties produced using FRP. So, the usefulness of this AS will be further enhanced if it could be extended to semi-batch conditions of sudden addition of initiator and sudden changes of temperature. In this work, we have shown that the AS with AK method can work quite well for both the semi batch conditions mentioned above. Another important aspect is that there are only three tunable parameters whose values are already available in literature. So, no tuning of parameters is done to match the curves. Still these values are found to be working well for semi-batch conditions. The AS results match excellently with the experimental data for the case of sudden addition of initiator [2] (Fig. 1a) and the sudden decrease of temperature [3] (Fig.1b). It also matches well against the results obtained through complete mathematical model with no assumption (FRP_Full) and one with Quasi steady state assumption (QSSA) for live radical polymer chains (FRP_QSSA). Thus, the AS can well replace the ODEs based mathematical model for FRP for all practical reactor conditions. Use of AS for process control for above mentioned semi-batch conditions seems promising.



(a) (b)

Figure 1: Semi-batch modelling result (a) for the case of sudden addition of initiator, (b) for the case of sudden decrease of temperature.

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Rakesh Guptha

TBD

Nanobubble modulated Amino acid Adsoprtion at Graphene Surface

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Surface nanobubbles are gaseous structures found at the interface between a solid and a liquid[1]. The exceptional stability of surface-attached nanobubbles is attributed to the pinning of the three-phase contact line and the hydrophobic attraction between the substrate and gas molecules. Despite their minuscule size, nanobubbles exhibit an astonishing range of characteristics, including a pronounced surface charge, exceptional gas transfer efficiency, and remarkable stability. These attributes render them neutrally buoyant, electrochemically reactive, and oxidative, making them invaluable players in domains such as oil & gas, waste-water treatment, drug delivery and surface cleaning. The present study evaluates the interaction behavior of nanobubbles with an amino-acid, namely alanine di-peptide, at the solid-liquid interface. It has been reported that surface nanobubbles promote protein stability[2] but the impact of surface characteristics on protein adsorption has not been studied in detail. Using molecular dynamics, we study how nanobubbles affect the adsorption of amino-acid on surfaces with different wetting characteristics, surface charges and electric potential. Figure 1 represents the potential of mean force profile for a nitrogen molecule surrounded by solvent for substrates with different solid-liquid contact angles. A hydrophobic surface is more conducive to the attachment and stability of nanobubbles than a hydrophilic surface thereby preventing the attachment of amino-acid on to the substrate. Our study establishes how behavior of amino-acids can be controlled using nanobubbles which provides an efficient and low cost design of biological devices with important implications for anti-fouling surfaces and protein storage.

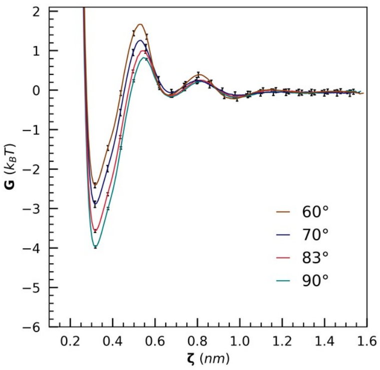

Figure 1: Potential of Mean Force of nitrogen molecule with substrates of different contact angle.

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Effective degradation of dark green rit dye using ozone nanobubbles

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Ozonation is seen as a beneficial approach since ozone is a strong oxidant utilized for disinfection, degradation, and elimination of organics, antibiotics, and microbes. Because of its fascinating characteristics, nanobubble technology has recently piqued people's interest. Here, we demonstrated our approach of combining ozonation with nanobubbles to enable efficient degradation of dark green rit dye wastewater. The effect of ozone nanobubbles on the degradation efficiency of dark green rit dye was studied at various pH levels. Ozone is produced in an ozone generator using the corona discharge method using a high purity oxygen from an oxygen concentrator. The results showed that raising the ozone flow rate increased the concentration of dissolved ozone. Wastewater was created by dissolving the required quantity of GRD in water. The solution was then placed in an acrylic tank, and the setup was run in recirculation mode with a diaphragm pump setup. The nanobubbles were created using an in-house nanobubble machine. A spectrophotometer (DR3900, HACH) was used to measure the left-over concentration at 526 nm. The results reveal that using ozone in the form of nanobubbles can destroy the dye in 3 minutes, as illustrated in figure 1 (a). Because direct ozonation occurs in acidic medium rather than basic medium, dye degradation is increased. Although degradation occurs in basic medium as well due to the generation of hydroxyl radicals. As a result, we can deduce that direct ozonation is favored at lower pH values, whereas indirect ozonation, which results in the generation of free hydroxyl radicals, is preferred at higher pH.

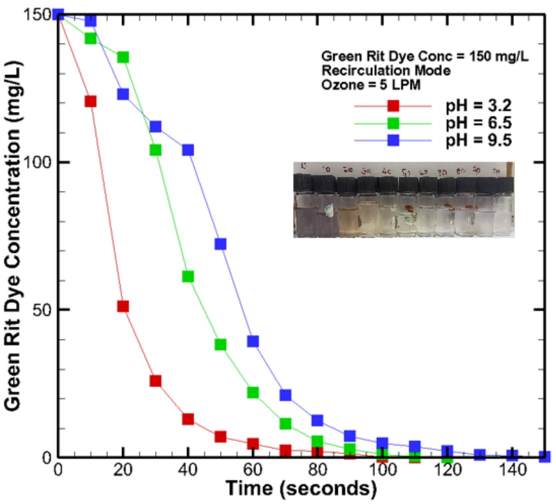

Figure 1: Degradation of green rit dye at various pH using ozone nanobubbles.

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Predicting Drug Release in Bilayer Osmotic Tablets: Model Development and Experimental Validation

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The Controlled Release System can be categorized into four types: Chemically Controlled, Diffusion Controlled, Osmotically Controlled, and Swelling-and/or Dissolution controlled. The Oral Osmotic pump (OROS) tablet, controlling drug release with osmotic pressure, offers advantages over other drug delivery systems. Advantages of OROS tablets include lower adverse reactions, improved compliance, reduced dosage, independence from hydrodynamic conditions, gastric pH, and agitation.

The first orally administered osmotic pump, known as Extrudable core system (ECS) or elementary osmotic pump (EOP), offers easy preparation and near zero-order delivery of water-soluble drugs. ECS has limitations with water-insoluble drugs as it can't fully extrude them once the osmotic agent is depleted. Bilayer systems like SCT resolve this issue, ensuring maximum drug extrusion.

This work presents a precise model for predicting drug release rate in bilayer osmotic tablets. Key parameters, including coating thickness, tablet size, excipients, and active pharmaceutical ingredient, are crucial for the model's precision. Efficient drug release of water-insoluble drugs at a controlled rate is the focus of this research. The model describes dynamically all the main release processes occurring during the dissolution of a tablet coated with a semi-permeable membrane, namely, the solvent influx driven by the difference in osmotic pressure across the coating in both drug and sweller layer, dispersion of core components (drug and polymer), swelling of the tablet due to solvent accumulation, build-up of hydrostatic pressure inside the tablet, tensile stress acting on the coating, and the efflux of the dispersed core components, dissolution of drug particles in bulk, swelling of the polymer in the sweller layer, and pressure exerted by sweller layer onto the drug layer. The model was validated by comparing the predictions with drug release data for three drugs with varying solubilities and for the same drug in different dissolution media. The predictions of drug release from SCT tablets are in good agreement with the measurements, suggesting that our model is well suited for elucidating the osmotically controlled drug release from SCT tablets.

Keywords: Osmotic controlled-release tablet, Swellable core technology, Osmotic pressure, Controlled drug release

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Indian Society of Rheology

Experimental investigations to study the drug release from bilayer osmotic tablets

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Controlled drug delivery systems, through the sustained release of drugs, enable the drug concentration to remain within the therapeutic range for a long time, thus increasing the effectiveness of drugs. One of the most successful delivery systemsis the oral osmotic delivery system, as the delivery of the drug is independent of external conditions such as pH and hydrodynamic conditions.

We have performed experiments on bilayer osmotic tablets in which the upper layer consists of a drug and polymer, and the lower layer consists of a swellable polymer and an osmotic agent (salt). Model (inert) particles were used instead of drug particles to understand the influence of various factors, such as orifice size and coating thickness, on the extrusion of the model drug particles. We have also designed a setup for collecting the extrudate to determine the relative ratios of polymer, osmotic agent, water, and drug in the extrudate and also to draw a comparison between these ratios and those existing in the upper layer of the tablet.To account for the reproducibility of the experiments, the experiments have been repeated twice for every time point. Next, we compared the measurements with predictions of a mathematical model that accounts for the details of the drug

delivery process, namely, solvent imbibition due to osmotic pressure gradient, hydration of the drug layer, swelling of the sweller layer, build-up of hydrostatic pressure, and extrusion of the extrudate through the orifice. The results show a good agreement between measurements and model predictions, suggesting that the model captures well all the key processes involved in the drug delivery process.

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Role of organic ligands on the gas adsorption and separation in Zeolitic Imidazolate Frameworks

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Metal organic frameworks (MOFs) are composed of metal ions that are linked via organic ligand molecules. They are porous and crystalline in nature with high surface area. There exists a wide range of linker molecules that can tune the properties of MOFs. This makes them a promising class of material for gas separations [1]. Towards this end, Zeolitic Imidazolate Frameworks (ZIFs), which is a subclass of MOFs resembling zeolite structure as shown for a representative case of ZIF-90 in Figure 1, exhibit reversible structural transformations such as breathing, swelling, and rotation of linkers responsible for variation in volume, surface area, and pore size, etc. [2]. Here, we combine grand canonical Monte Carlo simulation (GCMC), molecular dynamics (MD) simulation and density functional theory (DFT) to develop a deeper understand of ZIFs' flexibility and its impact on gas adsorption and separation. We estimate the adsorption isotherms for CO_2, N_2, CH_4, and H_2O in several ZIFs vis GCMC simulations. We predict the diffusion of gas molecules inside the ZIFs via MD simulation. Moreover, our DFT calculations provide energetically favorable orientation of gas molecules over the adsorption site. Our work provides important design rules of ZIF materials for gas separation application.

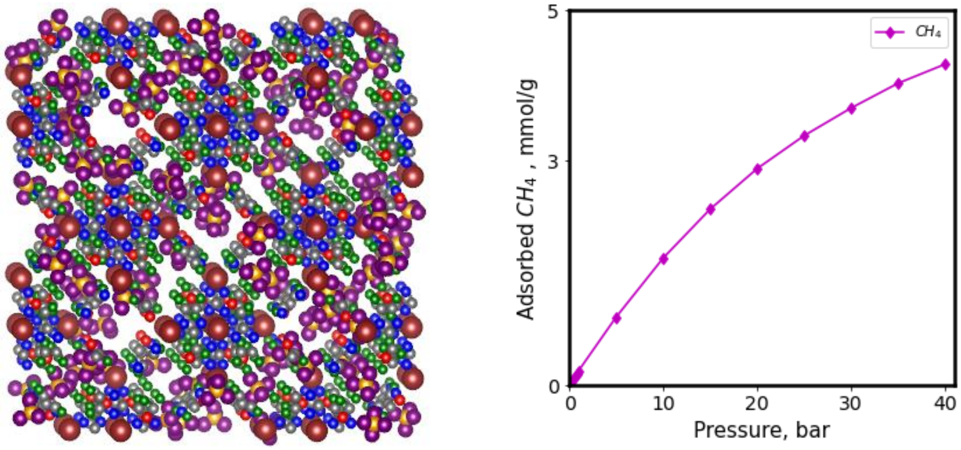

Figure 1: 2*2*2-unit cells ZIF-90, consists of zinc metal networking 2-carboxaldehyde imidazole as linkers (left), methane adsorption isotherm at 298 K (right). Carbon (grey), oxygen (red), hydrogen (green), nitrogen (blue), zinc (brown) and methane carbon (yellow), methane hydrogen (purple) are represented as spherical balls.

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Acoustophoresis-assisted Fluid Jet Polishing

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Fluid Jet Polishing (FJP) is a method of contouring and polishing a surface by aiming a jet of slurry from a nozzle and eroding the surface to create a desired shape. FJP finds its application in finishing micro-lens mold arrays, polishing microchannels, smoothing of micro-cusps, and generating functional surfaces. However, conventional FJP suffers from some drawbacks, such as a non-homogeneous erosion profile due to random particle impacts & formation of stagnation zone, unwanted erosion of the nozzle wall, and wastage of particles. Here, the acoustophoretic effect is being proposed as a possible means to overcome these drawbacks of conventional FJP.

Acoustophoresis is the process of manipulating the particles within a fluid stream by means of sound waves. The scattering of acoustic waves on the particles suspended in the liquid leads to momentum transfer from the sound field to particles giving rise to a 2nd order time-averaged acoustic radiation force, which results in particle migration. The main objective is to focus the impinging particles towards the center of the issuing nozzle so that we can get a "U" shaped erosion profile as opposed to the "W" shaped profile.

The numerical analysis has been performed using ANSYS Fluent Software. The geometry being modeled consists of a cylindrical nozzle and a circular target plate. The assumption of one-way coupling holds due to the small size & mass concentration of the abrasive particles. The fluid flow is solved using the finite volume method, and the particle tracking is done using the Discrete Phase Model (DPM). We investigate the erosion profile on the target plate for a variety of parameters, such as frequency of the input acoustic wave, Stand-Off distance, and inlet fluid velocity. We also analyze the erosion profile wrt different empirical erosion models present in the literature.

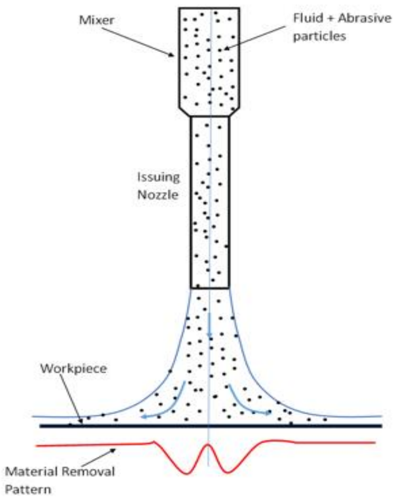

Figure 1(a): Erosion profile without acoustic forcing

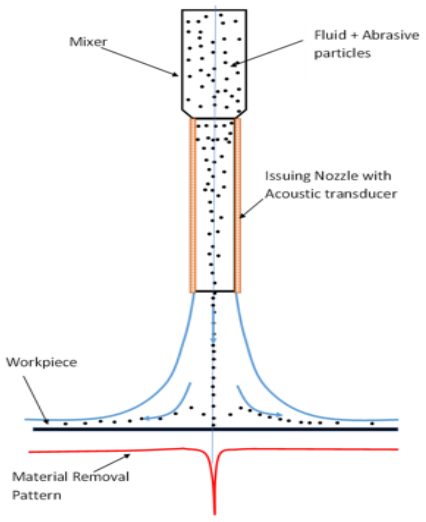

Figure 1(b): Erosion profile with acoustic forcing

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Nanobubble modulated Amino acid Adsoprtion at Graphene Surface

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Surface nanobubbles are gaseous structures found at the interface between a solid and a liquid[1]. The exceptional stability of surface-attached nanobubbles is attributed to the pinning of the three-phase contact line and the hydrophobic attraction between the substrate and gas molecules. Despite their minuscule size, nanobubbles exhibit an astonishing range of characteristics, including a pronounced surface charge, exceptional gas transfer efficiency, and remarkable stability. These attributes render them neutrally buoyant, electrochemically reactive, and oxidative, making them invaluable players in domains such as oil & gas, waste-water treatment, drug delivery and surface cleaning. The present study evaluates the interaction behavior of nanobubbles with an amino-acid, namely alanine di-peptide, at the solid-liquid interface. It has been reported that surface nanobubbles promote protein stability[2] but the impact of surface characteristics on protein adsorption has not been studied in detail. Using molecular dynamics, we study how nanobubbles affect the adsorption of amino-acid on surfaces with different wetting characteristics, surface charges and electric potential. Figure 1 represents the potential of mean force profile for a nitrogen molecule surrounded by solvent for substrates with different solid-liquid contact angles. A hydrophobic surface is more conducive to the attachment and stability of nanobubbles than a hydrophilic surface thereby preventing the attachment of amino-acid on to the substrate. Our study establishes how behavior of amino-acids can be controlled using nanobubbles which provides an efficient and low cost design of biological devices with important implications for anti-fouling surfaces and protein storage.

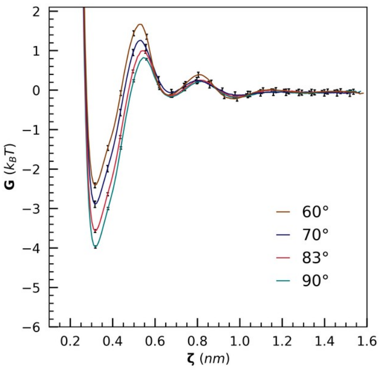

Figure 1: Potential of Mean Force of nitrogen molecule with substrates of different contact angle.

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Physics-Inspired Machine Learning for Multiphase Flow

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Abstract:
Euler-Lagrange (EL) and Euler-Euler (EE) techniques have been widely employed for solving particle, droplet, and bubble-laden flows. Since flow around the individual particles is not resolved, the accuracy of the technique depends on the fidelity of the point-particle force laws used. The main focus of this talk is the use of emerging machine learning techniques along with physical insight into the averaging processes involved in the EL and EE techniques can yield closures that recover fully-resolved-like accuracy at orders of magnitude lower cost.

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Complex flow behaviors of complex fluids in porous medium for applications in Energy industry

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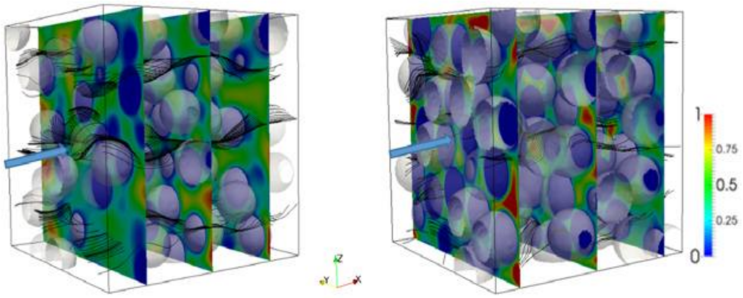
During the oil and gas recovery from subsurface, the recovery efficiency is mainly limited by two factors: pore-scale trapping resulting in irreducible hydrocarbon saturations and bypassing because of limited sweep efficiency due to rock heterogeneity, viscosity contrast and viscous instabilities. To improve the sweep efficiency, hydro-soluble polymer solutions with non-Newtonian rheology are applied. The difficulty is in predicting the in-situ effective viscosity in Darcy-scale flow in the porous medium, based on bulk rheology provided for instance by shear rheometers [1]. Most of the relevant polymer systems, however, also exhibit viscoelasticity which can lead to elastic turbulence during flow through porous medium [2]. Here we show progress on the fundamental side, how to visualize the respective pore scale flow fields and understand the fundamental origins using a system that contains one single pore throat [3] and multiple pore throats and its effect on residual oil saturation [4]. In addition, we demonstrate how we numerically simulate the flow of viscoelastic fluids in porous medium and characterize elastic turbulence [5].

In the field of CCUS and hydrogen storage similar complex pore scale flow behavior are also observed and the talk with also provide challenges and opportunities in such emerging research areas.



(a) (b)

Figure 1: Viscoelastic flow streamlines through a representative section of monodisperse spheres.

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Microfluidics Route to Generation of Biomaterials

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The Microfluidics and Nanomaterials lab in the Chemical engineering department at IIT Bombay has three thrust areas of research namely, 1) Microfluidics as a tool for generation of biomaterials; 2) Polymer nanocomposites for antimicrobial applications; 3) Development of Bio-inspired Food packaging materials. In this talk, I am going to focus on how we use Microfluidics as a tool for generation of Biomaterials. We develop various types of glass-based and glass-PDMS based microfluidic devices to fabricate biomaterials such as microparticles, microcapsules, and microfibers. These biomaterials are fabricated using various solidification techniques that include droplet coalescence coupled with chemical gelation[1] (Figure 1), electric field coupled with photopolymerization, and chemical gelation in the presence of electric fields, all implemented on-chip. The generated biomaterials are currently being used for biological applications such as eradication of biofilm, cancer biology and drug delivery, and water treatment.

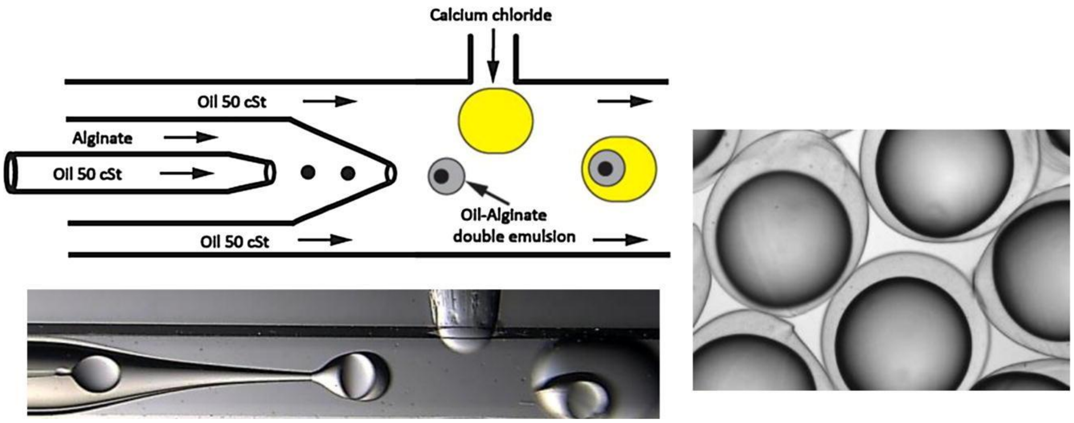

Figure 1. 3D glass-PDMS hybrid microfluidic device for fabricating oil-alginate microcapsules through chemical gelation and the generated capsules

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An altered streamline topology allows deformed drops to transport mass faster than spherical ones

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We analyze the effect of a drop-deformation-induced change in streamline topology on the scalar transport rate (the Nusselt number Nu) in the one-parameter family of ambient planar linear flows. The drop-phase resistance is assumed dominant, and the drop deformation is characterized by the Capillary number (Ca). For a spherical drop (Ca = 0), closed streamlines lead to Nu increasing with Peclet number (Pe), from a purely diffusive plateau for small Pe, to a second large-Pe plateau that arises due to transport being limited by diffusion across closed isothermal streamlines. A non-zero Ca destroys the closed streamline topology, and the flow field consists of spiralling streamlines densely wound around nested tori that foliate the deformed drop interior. For large values of PeCa, Nu increases beyond the aforementioned primary plateau, saturating in a secondary plateau that arises due to transport being limited by diffusion across nested tori. Even for arbitrarily small Ca, the secondary plateau is almost six times the primary one for planar extension, and nearly an order of magnitude larger for simple shear flow.

Next, we show that for a range of intermediate hyperbolic linear flows, where the zero-Ca streamline pattern exhibits both homoclinic and heteroclinic trajectories, the deformation-induced spiralling for small but finite Ca, is accompanied by chaotic wandering on longer time scales. We characterize the chaotic streamlines via the distribution of residence times in the different principal regions demarcated by the homo/heteroclinic trajectories at Ca = 0. We use these residence time distributions to extract the Ca-scaling for the time scale characterizing the chaotic wandering, and then correlate this time scale to a possible tertiary enhancement regime.

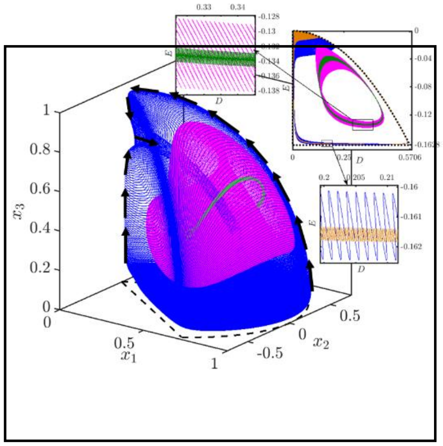

Figure 1: Finite-Ca streamlines in a deformed drop octant in a planar extensional flow

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Self-organized Microrhology of the Suspended Particles at the Mesoscale

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Abstract

Suspensions of mesoscale objects of diverse size and shape inside a fluid medium can self-organize under the influence of chemical or externally applied fields to develop novel microrheological properties. While a collection of glass beads can emerge localized pseudoplastic or dilatant behaviors inside a Newtonian fluid under the influence of an electric field, variations of the pH inside synovial fluid may engender protein segregation leading to the stiffness of the joints. In a way, all these processes have an inherent reversibility because such behaviors disappear once these influences are removed from the system. Notably, such behavior also emerges some fundamentally important phenomena such as asymmetric bridging and breaking of droplets under an electric field, creation of floating electrodes inside a liquid medium, among others. This talk explores some such examples covering both fundamental and applications associated with such phenomena.

Bio-Sketch

Dr. Dipankar Bandyopadhyay is a B.Sc in Chemistry and B.Tech in Chemical Engineering from Calcutta University. After completion of M.Tech from the Department of Chemical Engineering at IIT Kanpur, he served ANSYS - Fluent India Private Limited for more than 3 years as a CFD Engineer before completing PhD from IIT Kanpur. Presently, he is a Professor in the Department of Chemical Engineering and Centre for Nanotechnology as well as the Head of Jyoti and Bhupat Mehta School of Health Sciences and Technology, at IIT Guwahati. He is also one of the Directors of the R&D unit sponsored by Government of Assam at IIT Guwahati namely AAHII – Assam Advanced Healthcare Innovation Institute. Formerly, he has also served as the Head, centre for Nanotechnology IIT Guwahati. He has also served as visiting faculty at Yeungnam Univerisity at South Korea under the WCU Program, and KTH Sweden under the Erasmus Mundus program.

His research areas encompass Thin film Dynamics, Soft-matter Physics, Liquid Crystals and Smart Materials, Droplet and Digital Microfluidics, Health Care Point-of-Cater-Testing Devices, MEMS Theranostics, Microrheology, Clean energy, Computational Fluid Dynamics, Stability and Instability of Fluids, Complex Fluids, among others.

He has authored ~140 research publications in the international journals and has filed 23 Indian and 9 international patents so far. He is also one of the PIs of multiple Centre for Excellences at IIT Guwahati sponsored by MeitY, ICMR, and BIRAC. He is the recipient of NCL’s Prof. K Venkataraman CHEMCON Award in CHEMCON 2016. He and his group at the Indian Institute of Technology Guwahati is the recipients of Gandhian Young Technology award 2016 and 2019, BIRAC-SRISTI Appreciation Award 2017 and 2021. He is a nominated member of American Chemical Society, Royal Society of Chemistry, and Indian Institute of Chemical Engineers.

Dynamics of turbulence suspensions with inertial particles

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The particle transport is ubiquitous in natural processes such as fluvial sedimentation, dust storms, raindrop formation, and industrial processes such as electrostatic precipitators, mixing and coating, and combustion fuel. The presence of particle phase affects the length and timescales of turbulent flows. The prediction of these scales is necessary to capture the heat, mass, and momentum transfer properties across the turbulent flows, and the preferential concentration in low vorticity zones, turbophoresis induced particle clustering in near-wall for the particle phase. In the present study, large eddy simulations (LES) are performed for vertical channel flows to analyze the simultaneous dynamics of the fluid and particle phases. The fluid phase is resolved with the Eulerian approach, and the solid particles are tracked using the Lagrangian approach. The eddy viscosity-based LES models are observed to accurately predict the turbulence modulation at low-volume fractions. However, these models do not accurately capture the critical loading (CPVL) at which complete turbulence collapse is observed. A DNS study reveals that the local isotropy of small and large scales decreases in the near-wall and channel center with an increase in particle volume fraction and leads to the modeling error in LES models which are based on isotropic assumption. We performed simulations for different system sizes and Reynolds numbers to quantify the turbulence modulation. It is observed that the extent of turbulence attenuation increases with an increase in system size and decreases with an increase in particle volume fraction for fixed volume loading. It is also found that the Stokes number alone is not a correct parameter to quantify the effect of particle inertia on turbulence attenuation.

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Inertio-elastic orientation dynamics of anisotropic particles in linear shearing flows

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Anisotropic particle suspensions commonly occur in nature and industry. In making paper, cellulose fibre suspensions are processed in an aqueous solution, and the fiber orientation distribution, influenced by inertia, partly determines quality of the finished product. While suspensions of anisotropic particles in a non-Newtonian fluid traditionally occur in the context of filled polymeric materials, recent examples include active swimmers in a viscoelastic ambient. In the dilute limit, the rheology of such suspensions is governed by the behavior of a single anisotropic particle in an ambient linear shearing flow. When the particle is a spheroid immersed in simple shear flow of a Newtonian fluid, in the Stokes limit, its orientation vector rotates along any of a one-parameter family of closed (Jeffery) orbits on the unit sphere. Jeffery orbits are characterized by an orbit constant C varying from 0 to ∞. C=0 and C=∞ are the spinning and tumbling modes, respectively, with finite non-zero C corresponding to precessional motions (kayaking modes). The closed orbit configuration is structurally unstable, and even weak inertia or viscoelasticity therefore has a profound effect on the Stokesian orientation dynamics.

We investigate the orientation dynamics of a neutrally buoyant spheroid, with aspect ratio κ, in an ambient planar linear flow of a viscoelastic fluid. The particle Reynolds (Re) and Deborah (De) numbers, are assumed to be small but finite. No restriction is imposed on their ratio, the Elasticity number El=De/Re. We model the suspending fluid as a second-order fluid, introducing an additional parameter ϵ that determines the ratio of the normal stress differences. Using the reciprocal theorem, we obtain the inertial and viscoelastic torques as volume integrals involving the disturbance velocity field. Both inertia and viscoelasticity destroy the closed Jeffery topology. The resulting spiralling trajectory topology is quantified via ΔC, the change in the orbit constant in a Jeffery period, as a function of C. $\Delta C > 0 (< 0)\ \forall C$ leads to global stability of the tumbling (spinning) mode, while an intermediate zero crossing implies the existence of a limit cycle. A stable limit cycle implies convergence onto a kayaking mode for long times, while an unstable one implies partitioning of the unit sphere into distinct basins of attraction for the spinning and tumbling modes. The nature of the ΔC v/s C curves allows us to organize the inertio-elastic orientation dynamics on the κ-ϵ plane for different El and flow types.

For simple shear flow, for El →0 (dominant inertia), the tumbling mode is stable for prolate spheroids ($\kappa > 1$). While oblate spheroids with $0.14 \leq \kappa < 1$ approach the spinning mode, for those with $\kappa < 0.14$, the tumbling and spinning basins of attraction are separated by an unstable limit cycle. For El $\neq 0$, regions corresponding to unit-sphere trajectory topologies with stable and unstable limit cycles emerge from $\epsilon = \pm\infty$, moving inward with increasing El, on the prolate half of the κ-ϵ plane. On the oblate half, the region corresponding to a unstable-limit-cycle topology shrinks with increasing El, giving rise to a distinct region with a stable-limit-cycle topology above El ≈ 0.4. For El $\rightarrow \infty$ (dominant elasticity), a diverse range of orientation dynamics occurs across eight distinct intervals of ϵ. Next, this analysis is extended to the subset of planar linear flows where spheroids still rotate along closed orbits. We end with an analysis of rotation arrest, of spheroids of extreme aspect ratios, within a small De framework.

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Deterministic lateral displacement for precise microfluidic droplet sorting

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Deterministic lateral displacement (DLD) is a microfluidic technique that utilizes specific arrangements of micro-post geometry to separate objects larger and smaller than a critical diameter (*Dc*). The critical diameter is a function of the shape of the posts, the gap between the posts (*g*), and the relative shift between adjacent rows of posts, characterised by the row shift factor (ε), the ratio of lateral displacement in succeeding row to center-to-center distance between posts. We here present an experimental and theoretical investigation to analyse the dependence of different post shapes on the critical diameter of DLD ratchets. In particular, using a large set of simulations, we first derived a correlation to accurately predict the critical diameter in a DLD device with polygonal post shapes. To validate the correlation and experimentally determine the critical diameter, we used a novel approach to couple the DLD ratchet with an upstream droplet generator. The ability to precisely control the droplet size using a flow-focusing geometry allows us to accurately determine the critical diameter of the DLD geometry. Through comparison with experiments, we show that the proposed correlation can correctly predict the critical diameter with an error of less than 5%. Our experiments also motivate the use of DLD to improve the degree of monodispersity of an emulsion.

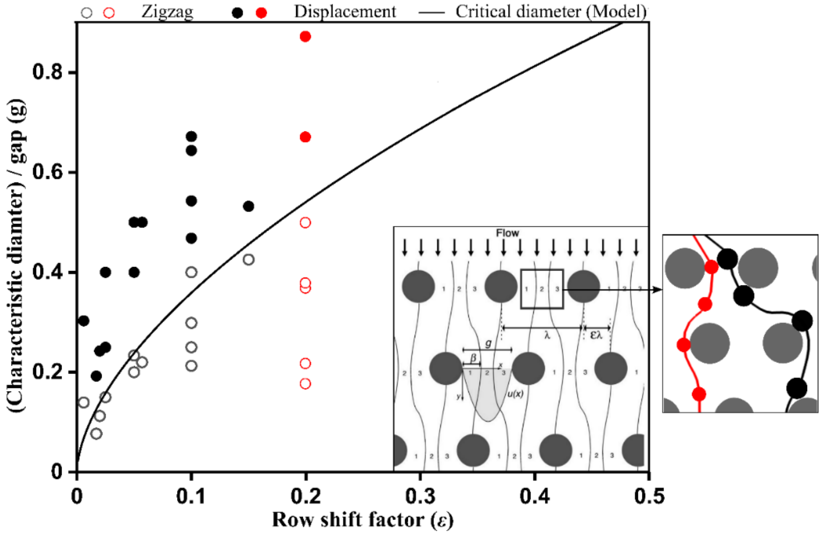

Figure 1: Dependence of critical diameter on the gap between posts and the row shift factor for circular posts. Solid points represent displacement mode and open points zigzag mode. In black (solid & open), particle diameter (literature) versus ε. In red, droplet diameter vs ε.

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Droplet Impact on Drone Propellers

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This study presents a comprehensive analysis of droplet impact on drone propellers, with an aim to understand their performance characteristics during rainy conditions. Experiments with varying droplet release heights and, thus, a wide range of Weber numbers were conducted. Impacts at different sections of the propellor blade were investigated. A frugal imaging technique was employed using a regular DSLR camera and an in-house developed microcontroller-based workflow. The study offers valuable insights into the effect of droplet impact on propeller efficiency and stability to assist in reliable operations in adverse weather.

Figure 1: Droplet impact on the static propeller at the mid-section of the propeller for droplets dispensed from three different heights (a) 20 cm, (b) 39.5 cm, and (c) 62 cm.

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Numerical analysis of the migration of a particle in a symmetric serpentine microchannel in inertial microfluidics

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Inertial particle microfluidics (IMF) is a relatively new technology that exploits inertial effects for the passive manipulation, focusing, and sorting of particles [1]. The presence of secondary flows due to flow-wise changes in the channel geometry can modify the number and location of the focusing positions and the length required for the particles focusing in the channel. The main forces acting on a particle are the inertial lift force, which aids in the particles focusing toward their equilibrium positions by acting perpendicular to the primary flow, and the secondary Dean drag force, which acts in the direction of the secondary flow. However, the specific impact of these forces on the migration of a particle within serpentine channels remains unclear. In this work, we numerically investigate the effect of secondary flow on the migration of a particle in a symmetric serpentine microchannel under mild inertia (Fig. 1). We employ an immersed-boundary-lattice-Boltzmann-finite-element solver to account for the fluid mechanics and particle dynamics and their coupling [2]. We consider a single particle and analyse how the inertial lift and secondary Dean drag forces act on the particle. Additionally, we study the effect of the particle size and Reynolds number on the particle equilibrium positions and focusing length. Understanding the focusing mechanism underlying particle migration will aid in designing and optimising inertial microfluidic channels.

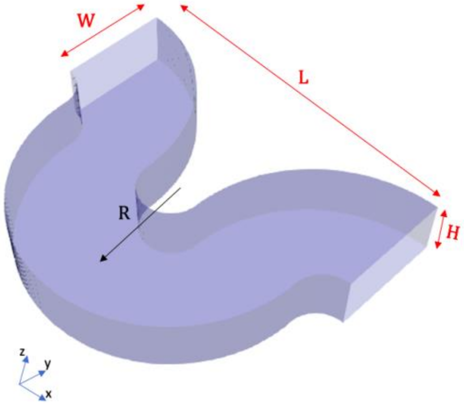

Figure 1: A symmetric serpentine microchannel geometry with height, H; width, W; and a periodic unit cell length, L

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Effect of size-disparity on the structure and dynamics of a Lennard-Jones mixture with random interactions between the particles

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The present work uses molecular dynamics simulation to investigate the structure and dynamics of a multicomponent fluid interacting via a Lennard-Jones (LJ) potential. The particles in the system are considered to be bidisperse in size and polydisperse in interaction energy. The polydispersity in energy is imposed by considering the particles to interact randomly, which is implemented by modifying the interaction parameter in the LJ potential. We analyze the microstructure of the systems at low temperatures by studying the radial distribution function and hexatic order parameter. We also analyze the transport properties like mean-squared displacement and intermediate scattering function in the vicinity of the liquid-solid transition temperature. Furthermore, the self-diffusion coefficient and the relaxation time are computed and analyzed.

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Influence of synthetic inflow perturbations on the dispersion characteristics of particles over a normal flat plate

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Understanding the dynamics of particle-laden flows is crucial due to their widespread significance in industrial, environmental, and biological applications, impacting various aspects of human life. Numerical simulation is a valuable tool for gaining insights into the behavior of particles suspended in laminar and turbulent flows. Realistic inlet boundary conditions are paramount for ensuring the accuracy of any numerical simulations. One effective technique for replicating real-world conditions in simulations is by introducing synthetic turbulent velocity fluctuations, which are superimposed on the mean velocity field. The primary focus of our study is to investigate how synthetic inflow perturbations influence the two-dimensional flow of a dilute particle suspension over a flat plate. Our main objective is to understand the impact of planar shear inflow, along with the introduction of synthetic perturbations, on particle dispersion in the wake and their deposition patterns on the plate. To achieve this, we utilize the in-house Eulerian-Lagrangian solver, MGLET-LaParT [1]. Using the solver we will investigate the one-way coupled interaction between Eulerian flow field and Lagrangian particle trajectories. By employing the synthetic-eddy-method [2], we can effectively introduce realistic fluctuations into the flow field, allowing us to study the intricate dynamics of particle-laden flows and their behavior under these perturbed conditions.

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Dispersion size measurement in multiphase systems using Depth from Defocus technique

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Particles dispersed in multiphase flows are ubiquitous across various natural and industrial applications, where the term ‘particle’ refers to discrete entities of any phase, including drops, bubbles, solid particles or even biomaterial. Characterisation of such systems involves extracting quantitative information such as the size, spatial location, velocity, and number density simultaneously, which is usually non-trivial. Unlike conventional methods, the ‘Depth from Defocus’ (DFD) technique offers an imaging-based volumetric approach for estimating the size and position of spherically dispersed particles from blurred projections. The two-image DFD approach [1-2] uses two cameras to capture simultaneous shadowgraph images at different degrees of blur, which requires a mandatory calibration procedure. Here, we develop a single-image DFD technique [3] that uses theoretical functions to measure size in a calibration-free manner. This enables in-situ experiments of difficult-to-measure composite fluid systems, including naturally occurring phenomena. To illustrate this technique, we examined various sparse spherical dispersions, including target dots, dispersed glass beads, liquid droplets, and pollen grains (Fig. 1). Furthermore, the method precisely determines the measurement volume, which ensures an unbiased estimate of size distribution and volume concentration. The straightforward optical configuration and semi-autonomous calibration procedure make this method easily accessible and deployable for diverse applications.

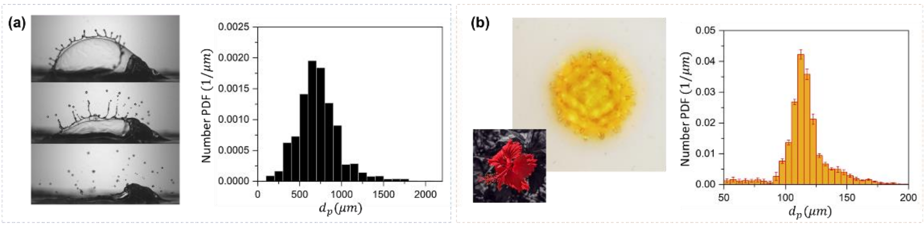

Figure 1: Measurement results depicted as Probability Density Functions (PDFs)
(a) Water droplets from surface bubble rupture (b) Dispersed pollen grains of Hibiscus

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Long- and short-time stability analyses of plane Poiseuille flow in an anisotropic porous channel

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The modal and non-modal stability of plane Poiseuille flow in a confined anisotropic porous channel is investigated. The channel is confined by solid impermeable walls and governed by the volume-averaged Navier-Stokes equation in the porous layers and the Navier-Stokes equation in the fluid layer. At porous-fluid interfaces, continuity of stress and velocity is employed, while no-slip conditions are used at impermeable walls. Note that the eigenvalue-based modal stability analysis only describes the asymptotic fate of the perturbation and thus fails to capture the short-term characteristics of the flow. In contrast, the non-modal stability analysis determines the perturbation response over a short time and the transient growth of the perturbations. The present study shows that the system parameters, such as porosity, anisotropic permeability, and porous layer thickness, significantly affect the short-time stability characteristics of the flow that lead to transient energy growth. The present analysis provides a valuable means to control the flow instability of a multi-layer porous system with anisotropic permeability.

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A minimal continuum model of clogging in spatio-temporally varying channels

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Particle suspensions in confined geometries exhibit rich dynamics, including flowing, jamming, and clogging[1]. It has been observed that jamming and clogging in particular are promoted by variations in channel geometry or fluid material properties[2] - such variations are often present in industrial systems (e.g. local confinements) and biological systems (e.g. stiffening of red blood cells in deoxygenated conditions in sickle cell disease). The aim of this talk is to shed light on the macroscopic dynamics of particulate suspensions in these conditions. To this end, we present a continuum two-phase model of particle suspensions that accounts for spatio-temporally varying material properties or channel geometries. The model comprises a continuous particle phase which advects with flow and has material properties dependent on the particle volume fraction, and a suspending fluid which flows through the particle phase obeying Darcy's law. We solve the system using the method of characteristics and simulate the evolution of an initially uniform particle density. We find that varying material properties and varying geometry can induce heterogeneity in particle volume fraction. We are able to show the emergence of high and low particle density regions and complete clogging of the particle phase in both pressure-driven and volume-driven flows. These results clarify how spatial variation in material and channel properties can contribute to clogging of particle suspensions

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Modeling droplet decisions in 1D microfluidic networks

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Droplet microfluidics deals with the generation and manipulation of droplets in a continuous phase medium flowing through an engineered microchannel. This phenomenon is used for various practical applications such as mixing, synchronization, and encapsulation in a lab-on-chip device. A microfluidic network consists of several interconnected flow channels[1]. The flow of droplets through these networks is more complicated than that of just a single-phase flow. Droplets flowing through a network make decisions about choosing a branch whenever they reach a node interconnecting two or more channels. In this work, we tried to use a network model[2] to experimentally demonstrate the decision made by drops in a loop device, which is the simplest form of a network. Experiments were conducted on a device made of PDMS with aqueous droplets as the discrete phase and silicone oil as the continuous phase. We observed that the droplets make different decisions for the same droplet configuration and topology over time. We aim to develop a robust model which will be able to predict droplet decisions more precisely. A simulation based on the existing model for the same topology and conditions was developed and run. The experiment and simulation data were compared, and the model was modified to predict droplet decisions with greater precision. This modified model will be helpful in practical applications that require precise manipulation of droplet decisions in 1D microfluidic networks.

Keywords: Microfluidic network, loop device, droplet decisions

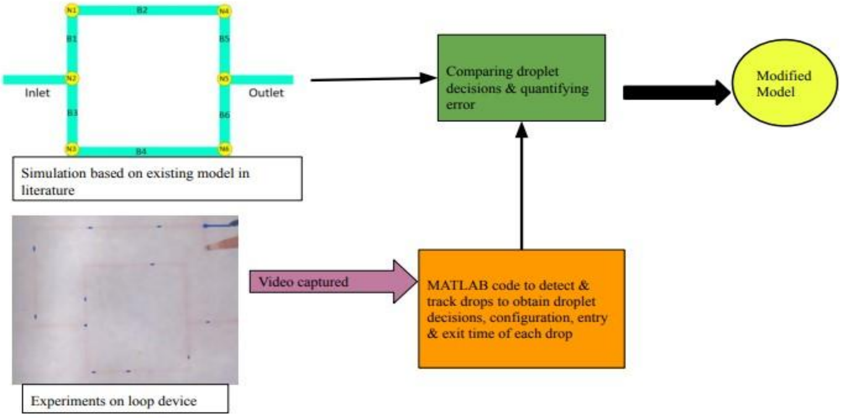

Figure: Schematic representation of the workflow

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Elastohydrodynamic Of Faraday Instability

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The natural frequency of a fluid layer overlying on a rigid wall depends on the density of the fluid, surface tension at the free surface and the waveform that evolves at the free surface.However, the presence of a soft-gel layer underneath the fluid layer is expected to alter the natural frequency of the fluid layer. In this work, a linear stability analysis is carried out to show that the natural frequency of the fluid layer is altered by the elasticity of the compliant soft-gel layer. As a consequence of a shift in the natural frequency, linear stability calculations shown that there is also a shift in the instability regions when the fluid layer lying on the soft-gel is subjected to Faraday forcing. This indicates that the soft-gel layer either has a stabilizing effect or a destabilizing effect because the presence of a deformable soft-gel layer either raises or lowers the Faraday threshold to induce an instability.

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Thermodynamic Effects on Viscous Fingering

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Viscous fingering (VF) accompanied by finger-like patterns is an interfacial instability which occurs when a more viscous fluid displaces a less viscous fluid in a miscible two-fluid system. Recent experiments have shown (*Suzuki et. al. (2019, 2020))* topological changes in VF when partially miscible system is considered. It is believed that due to spinodal decomposition induced by the thermodynamic instability where the second derivative of the free energy with respect to the composition is negative in binary mixture *(Mauri, Shinner & Triantafyllou 1996)*, the fingers developed fragments into droplets. *Seya et. al (Seya 2022)* presented numerical investigation of the same considering a simple thermodynamic free energy and including the Korteweg force effect, which replicated the experimental results.

Spinodal decomposition occurs when the enthalpy of the system, H = $\Psi\phi(1-\phi)$ present in the Gibbs free energy, G = H – TS is positive and sufficiently large to overcome the entropic stabilization and drive the phase separation process. Ψ is known as the Margules parameter, which is associated with the interaction of molecules in the system. In general, the unstable state is reached when Ψ exceeds a critical value. Larger values of Ψ influence the chemical potentials and concentration gradients driving the phase separation. Hence, our objective in this study is to investigate the effect of Margules parameter on the phase separation process in binary mixture and the underlying physics involved. We solve modified Hele-Shaw-Cahn-Hilliard (HSCH) model involving continuity, momentum, mass transport and the Cahn-Hilliard equations.

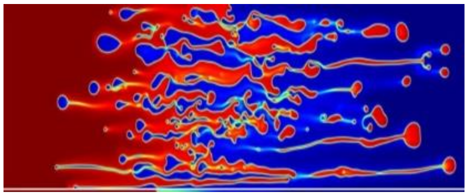

Figure 1: Concentration field at dimensionless time, $\tau = 4000$, for Margules parameter, $\Psi = 2.2$.

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Hydrodynamic stability of gravity waves on a free surface: Effect of curvature

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Surface gravity waves are ubiquitous in nature. These waves play a vital role in the dynamics of the ocean, such as the transport of micro-particles, organic material and for commercial purposes such as power generation. The air-water interface has a huge density contrast, and the kinematic viscosity of water is lesser than that of air, thus often allowing one to study such problems assuming the interface to be a free surface. In this study, we study the growth of waves in a shear flow bounded between a rigid wall and a free surface using linear stability analysis and characterize the instabilities in the system. The base state shear flow in water is chosen as a one-parameter family of quadratic velocity profiles, allowing us to access unidirectional and flow-reversal profiles. We perform both viscous and inviscid instability calculations for this family of shear flows using exact analytical, longwave asymptotic and numerical methods. Our study highlights the four kinds of instabilities in the system [1]:

- An inviscid rippling instability [2]
- A viscous longwave interfacial instability - a modified Kaptiza instability [3]
- A viscous Miles instability [4]
- A viscous Tollmien-Schlichting instability [5]

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Nonlinear evolution of a Dewetting bilayer thin film on a soft-gel layer

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The nonlinear evolution of Dewetting bilayer thin film on a soft-gel is investigated in this work. The fluids are considered to be Newtonian and the soft-gel layer in modelled as a liner viscoelastic solid. The free surface of the top fluid is exposed to air. The van der Waals attractive forces between the soft-gel layer and the fluids are the primary driving forces responsible for the rupture of the thin films. Short range repulsive forces play a key role in the dynamics of the system for very thin bilayer. Linear stability analysis of the system confirms two long wave instabilities one the liquid-liquid surface and other at the free surface arise in the system. The liquid-liquid (interface) instability is dominant when the attractive forces between the soft-gel layer and the bottom (top) fluid are strong. For a range of parameters both instabilities coexist in the system. The short range repulsive forces can suppress both these instabilities. The soft-gel layer has a destabilizing effect on the long wave instabilities.

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Phase separation of binary liquid confined inside uniform pore with wetting effect

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Exploring the intricate dynamics of phase separation in a confined cylindrical pore with wetting influence, this work delves into the fascinating phenomenon of binary fluid phase separation and its implications for various industrial and scientific applications. Unlike existing studies that suggested complete phase separation is unattainable within cylindrical porous media, our realistic model incorporates fluid-wall particle interactions. By implementing our model, we successfully achieved complete phase separation, presenting a significant advancement in understanding this phenomenon. Our numerical analysis explores the phase separation process under varying wetting strengths, pinpointing the critical threshold where partial wetting transitions to complete wetting. Predominantly we investigate the growth of the domain length scale and determine the growth exponent for all the cases, shedding light on the underlying dynamics of this intriguing phenomenon, which shows different behavior with different strength of interactions. Distinct growth exponents are exhibited by various particle types once transitioned to complete wetting regime. To provide further justification and explanation for these findings, we employ the structure factor, leveraging the Porod law and Super-universality principle.

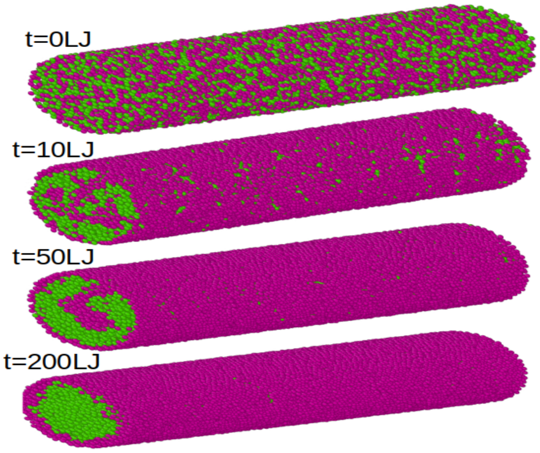

Figure 1: Evolution snapshots of complete phase separation obtained in the cylindrical pore with wetting strength corresponding to complete wetting.

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Film Dynamics Over a Topographical Surface Using Lattice Boltzmann Method

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In this work, the dynamics of a spreading liquid film on a planar and topographical substrate are numerically modeled using the phase-field lattice Boltzmann approach (PFLBM). A two-phase interface is inherently mesoscopic in nature, making the PFLBM a suitable technique for modeling. Interfacial patterns generated using PFLBM perfectly match the experimental and analytical results obtained within the lubrication assumption. PFLBM simulations uncovered that steady-state solutions are not possible for large topographies and the fluid-fluid interface results in a series of droplets, leaving the topographical feature in the downstream direction. A decrease in viscosity ratio (bottom to top fluid) increases the height of the capillary ridge formed, making the film more prone to instability. We also explore the effect of multiple obstacles on the capillary ridges formed by each and obtain the condition of independent obstacles. Finally, a detailed analysis will be presented for the effect of aspect ratio (film thickness away from contact point versus capillary length) on planar surfaces with contact-line spreading. Our study unveils that at a critical value of the aspect ratio, the maximum value of dimensionless capillary ridge height reaches unity, and this critical value is found to be independent of the inclination angle. On further increasing the value of this parameter, a nose-like structure appears near the contact point, which is strongly dependent on contact angle values.

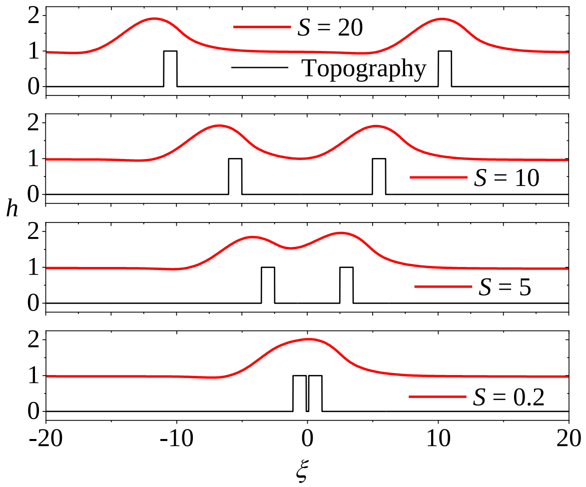

Figure 1: Effect of the obstacle location on the interfacial pattern formed by a thin liquid film using lattice Boltzmann method.

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Clustering and chaotic motion of inertial particles in an isolated vortex

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Inertial particles sample a flow field preferentially, getting centrifuged away from vortical regions and accumulating in strain-dominated regions. The dynamics of heavy particles in an axisymmetric vortex monopole are along expected lines - particles spirally migrate to infinity. We show that a deviation from axisymmetry for the vorticity profile can lead to intriguing clustering dynamics for inertial particles. We consider the Kirchhoff's vortex [1], an elliptical patch of uniform vorticity that rotates with a constant angular velocity, and show that four fixed points exist for heavy particles in the irrotational exterior. They appear as saddles and stable spirals, and we investigate their stability as a function of the Stokes number. A background shear often strains elliptical vortices - the Kida vortex is an example. Beyond a critical shear rate, the Kida vortex is known to exhibit Lagrangian chaos; the tracer pathlines are chaotic [2]. We study the dynamics of heavy inertial particles in a Kida vortex, investigating how particle inertia can compete with background shear to suppress the occurrence of chaotic trajectories. We find that the absence of a background shear will result in regular dynamics of inertial particles leading to a smooth basin of attraction (Figure 1(a)). In contrast, the background shear will induce chaos to the particles resulting in fractal basin boundaries (Figure 1(b)). We present a detailed theoretical and numerical study to evaluate the critical inertia of the particles to be immune to this shear-induced chaotic dynamics.

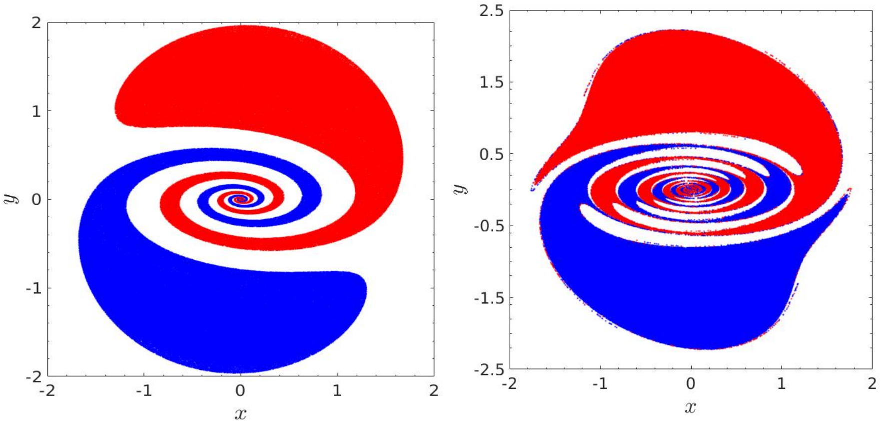

Figure 1: The basin of attraction of small inertia particles in Kirchhoff's vortex when (a) no external shear flow, and (b) in the presence of an external shear flow. The different colours indicate the basins correspond to different attractors.

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Effect of Vicsek like activity on the Vapour liquid phase separation inside cylindrical nanopore

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The separation of vapour-liquid mixtures from non-equilibrium high free energy state (homogeneous phase) to an equilibrium low free energy (particle rich and particle poor phase), while under various constraints, is a complex non-linear process that is not fully understood. In this work, we present our findings on the influence of Vicsek-like activity on the growth dynamics of vapour-liquid droplets, when constrained within a quasi-one-dimensional structure. Our investigations delve into the structure and growth dynamics under different levels of Vicsek interaction strength, providing a comparative analysis with passive limits. Existing research posits that, achieving complete phase separation within that restrictive structure is improbable. However, our novel model challenges this assumption, demonstrating the possibility of full phase separation. Our findings reveal that both the correlation function and structure factor obey dynamical scaling, which signifies the fact that coarsening patterns are statistically self-similar in time. We have also probed the applicability of power law in the domain growth kinetics and aging dynamics, which serve as key components for understanding such non-equilibrium systems.

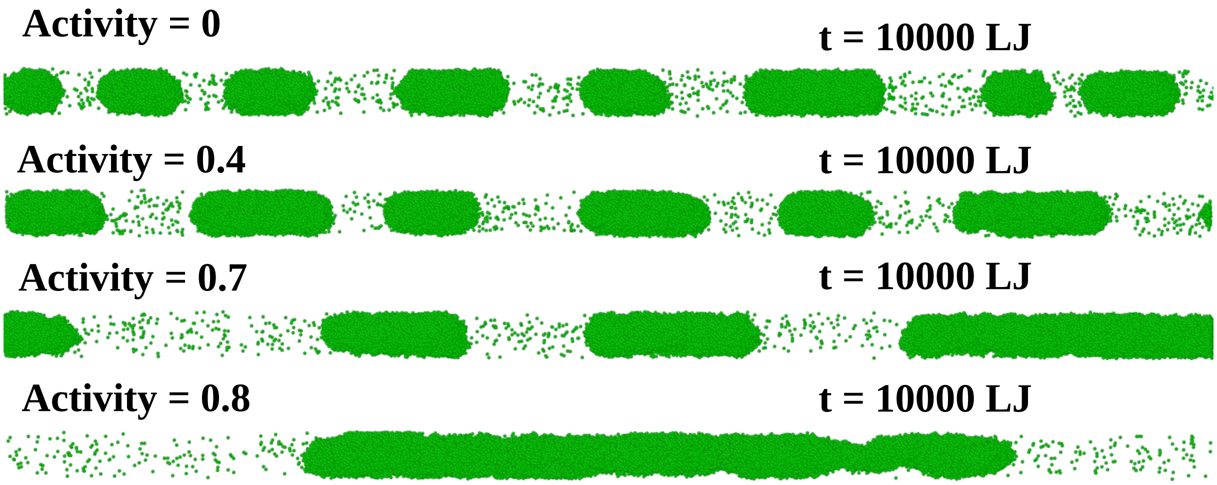

Figure 1: Snapshot of the system with different activity

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Enhancement of Chemical Reactions using Droplet-Based Microfluidics: A Study on Contact Modes and Reaction Kinetics

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In recent years, droplet-based microfluidics (DBM) has become a powerful platform for conducting various chemical reactions due to its ability to manipulate small amounts of liquid with high precision. The present work analyses the impact of two contact modes, Conjugate Mass Transfer Mode (CMTM) and Single-Sphere Mode (SSM), on different reactions occurring in droplet flow. Two reaction networks, Parallel reactions (PR) and Series-Parallel reactions (CR), are analyzed. These reaction schemes involve reactants A and B, forming a mixture of products of which only one is desired (D). The first contact mode, CMTM, involves the mass transfer of one reactant from the Continuous phase (CP) to the Dispersed phase (DP). In contrast, in the second mode, SSM, both reactants coexist within the dispersed phase, facilitating reaction and mixing inside the droplet. The Hadamard-Rybczynski flow field is used to get insights into the system's behavior. Our approach helps identify optimal conditions that determine the favorable contact mode for the system. The performance depends on the feed concentration ratio (M) and rate constant ratio (kr). This study showed that, in CMTM, the initial concentration ratio of A and B significantly affects the optimal conditions of desired product formation, and the optimal choice of this value depends on the type of reaction kinetics. On the other hand, SSM with an equal initial concentration of A and B results in a higher formation of the desired product (D) for all reaction schemes studied.

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Evidence of an inertialess Kapitza instability due to viscosity stratification

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We investigate the linear stability of a flow down an inclined plane in the inertialess limit, focusing on exploring different models of viscosity-particle concentration relationships. Here, we use a long-wave asymptotic analysis and a Chebyshev collocation based spectral method to investigate the stability of the film under various scenarios. By considering different models of viscosity-particle concentrations, we gain critical insights into how variations in these relations impact the stability of the film. Our findings indicate that viscosity stratification, occurring due to shear-induced migration in dense suspensions, can lead to instability in the Stokesian regime[1], which otherwise is impossible in the particle-free scenario[2,3].

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Quantitative measurements of immiscible oil jet

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The frequency of underwater oil-well blowouts in deep oceans has significantly increased due to the expanding offshore oil recovery and exploration activities. After a blowout occurs, a high Reynolds number crude oil jet forcefully emerges from the source and undergoes fragmentation, forming droplets. These droplets mix with the surrounding water, interact with various oceanic layers, and eventually rise to the ocean's surface. However, the opaqueness of crude oil poses challenges in examining the flow characteristics of these immiscible jets and plumes [1]. To address this issue, the present study employs a liquid-liquid pair with a refractive index matching technique using silicon oil and sugar water. These fluids possess properties comparable to those of crude oil and seawater. The use of refractive index-matched fluids enables the investigation of the jet's flow field and facilitates quantitative measurements [2]. The study involves conducting Particle Image Velocimetry (PIV) experiments on both single-phase water jets and immiscible oil jets at various Reynolds numbers. The PIV data provides information on the centerline velocity and half-width, allowing for a quantitative assessment of jet spreading in the oil jet, which is then compared with the single-phase water jet. The results demonstrate that the calculated jet half-width differs between the single-phase and multiphase jets. Furthermore, the radial velocity profiles of oil jets exhibit a self-similar behavior. Planar Laser-Induced Fluorescence (PLIF) experiments are carried out to visualize the boundaries of the oil jet and oil droplets. A significant finding of this study is the formation of compound droplets following the primary breakup. The instability of the shear layer and the subsequent engulfment of the oil and water layers are identified as the key factors responsible for the formation of compound droplets.

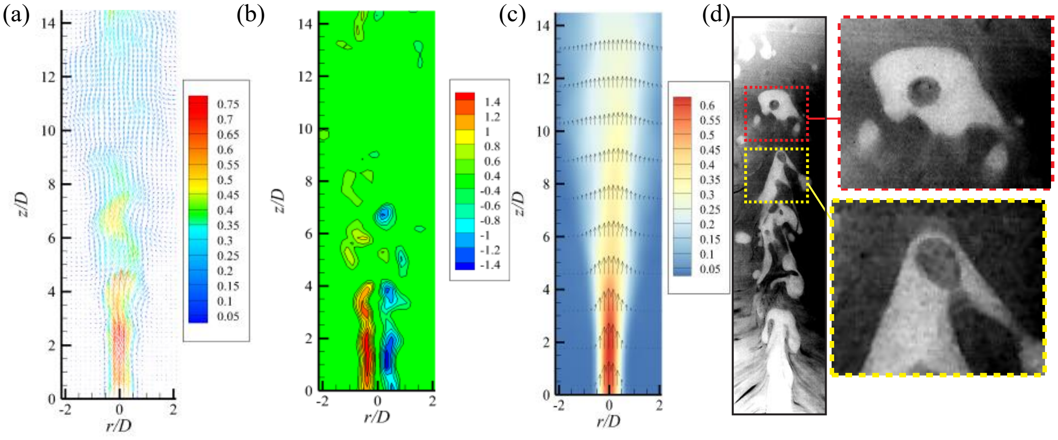

Figure 1: PIV and PLIF of silicon oil jet in sugar water at *Re* = 560. (a) Instantaneous velocity vectors. (b) Instantaneous vorticity contours. (c) Mean velocity magnitude with superimposed velocity vectors. (d) PLIF images showing oil and water phases with insets showing compound droplets

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Weakly nonlinear analysis of flow driven morphological instability in porous anodic oxides

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Porous anodic oxide on the metal surfaces formed as a result of electrochemical oxidation of metals in acidic solutions. The optimum parameter choice results in the formation of hexagonally organized submicron pores within these films. This porous anodic oxide plays a vital role in various industrial applications, particularly in the advancement of functional nanodevices. In this study, we investigate a weakly nonlinear analysis of the model by advancing beyond the stability threshold to determine the nature of instability. A linear stability analysis elucidates the underlying physical mechanism responsible for the selection of wavelengths. Anion adsorption on surface growth sites causes nonuniform compressive stress at the oxide and solution interface, which induces the flow. The competition between destabilizing viscous oxide flow and stabilizing oxide formation determines the length scale for the inter pore spacing. The results of the weakly nonlinear analysis of flow-driven growth mechanism of porous anodic films show that the solutions emerging from the critical state are supercritical for the entire range of investigated control parameters as shown in Figure 1

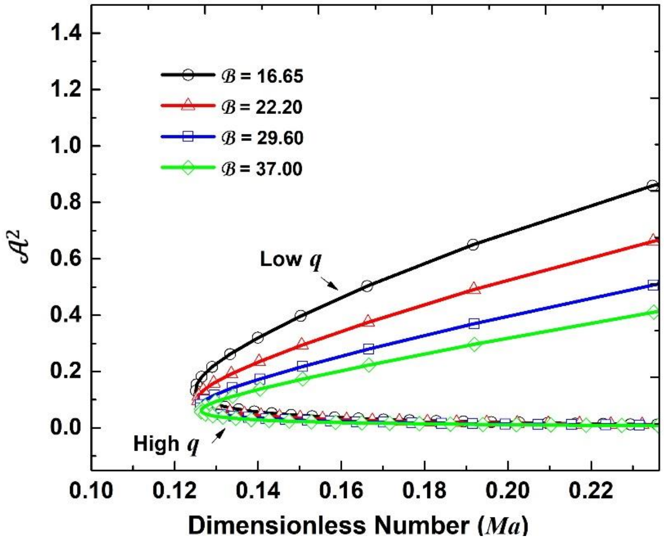

Figure. 1 The order parameter $\mathcal{A}^2$ vs. effective Marangoni number (Ma) for different values of high field conduction parameter $\mathcal{B}$, obtained from weakly nonlinear analysis.

Vorticity generation in miscible, volatile film spreading.

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In this study, we unveil an intriguing mechanism of vorticity generation driven by surface tension beneath a rapidly expanding ethanol-water film. This film forms atop a deep water layer upon deposition of a millimeter-sized ethanol-water droplet onto the water's surface. Usin particle image velocimetry, we investigate the evolution of vorticity beneath the expanding film. Remarkably, we discern a continuous increase of vorticity, increasing in the form of an expanding vortex ring expanding in the water layer below the film's periphery. This escalating vorticity progression leads us to hypothesize an ongoing vorticity generation at the fluid interface. To explain the observed phenomenon, we propose a novel model for vorticity generation based on a tangential surface tension gradient at the interface. Our model shows that the vorticity generation at any instance shows a power law dependence on time as $\omega_g \sim t^{-0.75}$, showing dependence on other drop properties. The dimensionless mean total vorticity at a given time instant is then shown to vary as $\omega_T^* \sim t^{*0.25}\xi^{0.75}$, where t^* is the dimensionless time and ξ is the drop viscosity ratio.

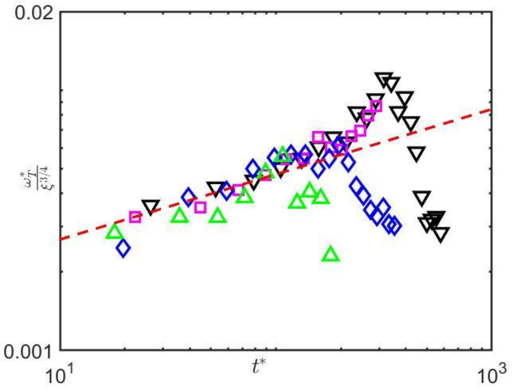

Figure 1: Dimensionless mean total vorticity vs dimensionless time.

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DYNAMICS OF PARTICLES IN LINE PLUMES

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We present a study of particle dynamics in line plumes with a uniform heat flux **Q** at the source to observe dust free regions with these plumes. We obtain a novel dimensionless form of the Maxey-Riley equation of particle motion by including thermophoretic force and normalizing the equation with the near wall length scales of Townsend, 1958. The particle motion is shown to be dependent on the modified Stokes number ($\mathbf{St_m=0.5(2+\varepsilon)C_BSt}$), the flux Rayleigh number ($\mathbf{Ra_f= (g\beta y^3Q)/(\vartheta\alpha K_f)}$), the flux-thermophoretic number ($\mathbf{Th_f=(2C_BC_TPrQ)/(T_pK_f)}$), the Prandtl number (**Pr**) and the gravitation number ($\mathbf{Gn=((1-\varepsilon)C_BSt)/Fr^2}$). The dimensionless plume velocity fields are obtained from the similarity solutions of Gebhart, using the same near wall length scales. We then solve the dimensionless Maxey-Riley equation numerically, subjected to this plume velocity field to obtain the flow streamlines and the trajectory of the particles. Dust free regions are observed at the center line of the plumes at larger $\mathbf{Th_m}$.

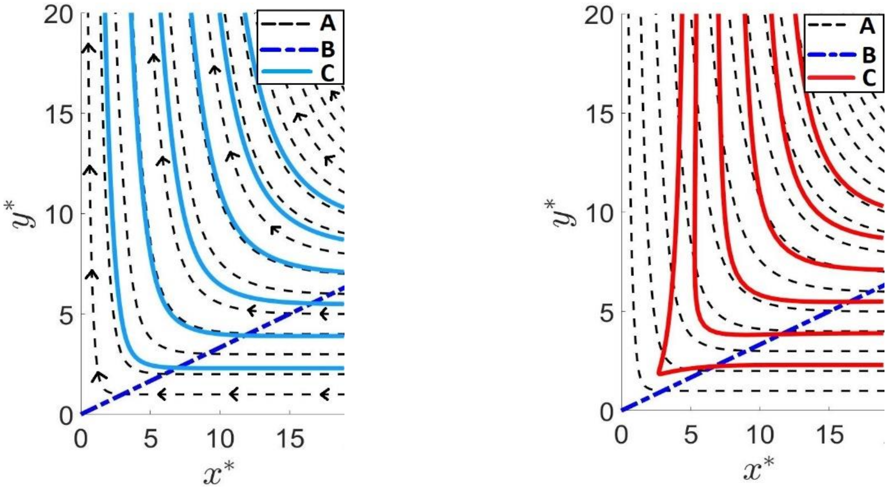

Figure 1: The left figure shows flow streamlines and particle paths at Pr=0.7; Gr_g=10; $St_m=10^{-5}$; Gn=0; Th_m=0. The right figure shows flow streamlines and particle paths at Pr=0.7; $St_m=10^{-5}$; Gn=0; Th_m=0.3; A = flow streamlines, B = Boundary layer edge, C = Particle trajectories.

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Determining the flow fields near a moving contact line: comparison between experiments and theory

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A moving contact line occurs when an interface separating two immiscible fluids meets a moving solid as shown in figure 1(a). Theoretical models in the viscous regime, first pioneered by Huh & Scriven [1], while suffering from a singularity at the contact line, make predictions of the flow fields. In particular, the theory predicts two broad types of flow fields depending on the viscosity ratio ($\lambda = \mu_A/\mu_B$) and dynamic contact angle ϕ. The Huh & Scriven model also forms the basis for more sophisticated models and the flow fields predicted in [1] retain their structure in advanced models. The present study is the first of its kind where systematic comparison of flow fields and interface shapes is carried out. Most of the earlier comparisons are often restricted to comparing only the dynamic contact angle.

The present study involves obtaining flow fields using particle image velocimetry (PIV). The probe the flow fields near a moving contact line, a 5X zoom lens is fitted to a high-speed camera. Viscosity is varied by using different grades of silicone oils ranging from 5cSt to 500cSt. Seeding the flow is done using $5\mu m$ polyamide particles. Flow fields and interface shapes are extracted from the images using standard PIV algorithms and compared with theory. Since the interface is always curved in the experiments, we adapt the model of Chen et al. [2]. We also provide detailed comparison for interface shape obtained from our experiments with theoretical models of Dussan et al. [3] and Chan et al. [4]. Figure 1(b) shows a sample comparison of the streamfunction from experiments and theory.

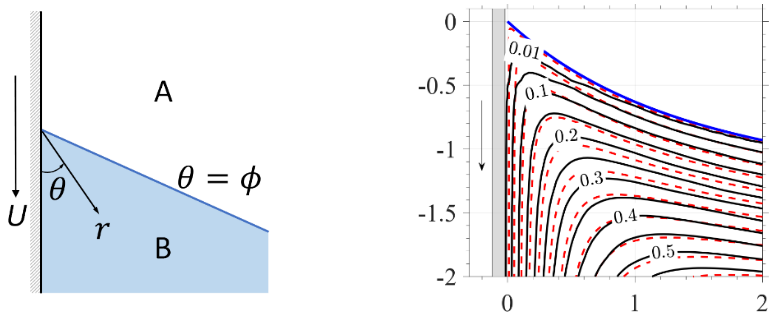

Figure 1: (a) Schematic of a moving contact line, (b) comparison of streamfunction between experiments (solid) and theory (dashed) for 100cSt silicone oil with $Ca = 4.57 \times 10^{-3}$.

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Behavior of Confined Gas Bubble and Liquid Droplet in Liquid Co-Flow.

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The dynamics of bubbles/droplets traveling in a confined geometry attracts attention from a diverse range of research fields including transportation of gas and liquids through pipelines, enhanced oil recovery and flow through porous media, medical therapy, microfluidic heat and mass transfer, conventional extraction [1]. This study numerically compares the behavior of a single bubble/droplet through a vertical channel with an imposed external flow (both upward and downward liquid flow). While gas-liquid systems were extensively studied earlier, studies on a droplet subjected to an external flow in presence of buoyancy effect are scarce. The interplay of Buoyancy, capillary, viscous forces along with the external flow significantly affects the bubble dynamics. This work aims at understanding the effects of different forces in terms of dimensionless numbers such as the Bond number (Bo), the capillary number (Ca), and the Reynolds number (Re) for different density ratios. In this study, an inhouse solver based on the Level Set Method is developed and employed for capturing the inter-fluid interface. The model developed is validated with standard test problems from literature. Preliminary simulations indicate a higher bubble rise velocity as the Ca is reduced, at a constant Bo and Re. This is depicted in Fig 1c. Fig 1 a depicts the droplet position and shape for different Ca and Fig 1 b represents the internal circulations developed within the droplet. Further, the effect of Bo, Ca, and Re is thoroughly investigated for medium size droplet/bubble for a range of Ca (0.001 – 0.5), Re (1-1000) and Bo (1-50). Thus, this study can provide insights into how different forces influence the movement and interactions of bubbles and droplets in pipelines, leading to more efficient and controlled transport processes. In medical applications, such as drug delivery and targeted therapies, the behavior of microbubbles and droplets within the body is relevant. This research could aid in designing methods to control the movement and distribution of therapeutic agents, potentially leading to more effective medical treatments.

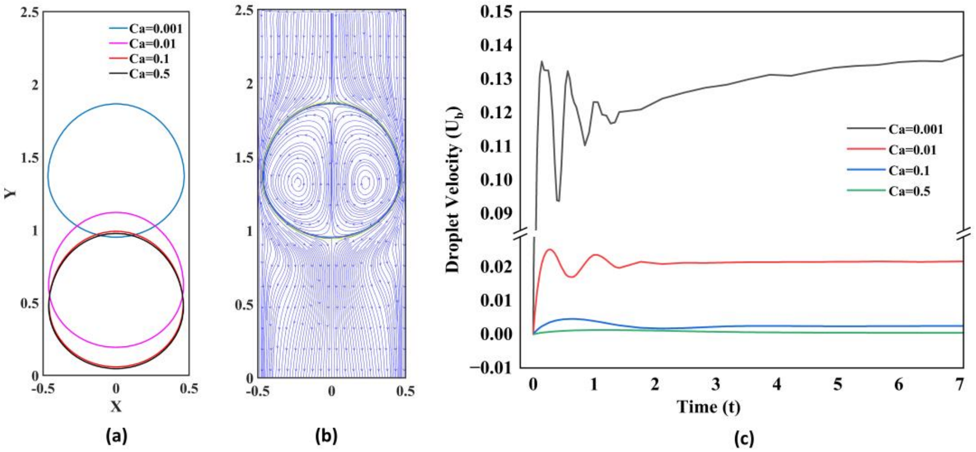

Figure 1: a) Effect of Ca on steady state shape and position of droplet rising in liquid co-flow with initial diameter D=0.925 **b)** Steady state velocity profile of a droplet rising in liquid co-flow with Ca=0.001 **c)** The effect of Ca on droplet translational velocity.

References

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An Experimental Study of Streaming Patterns Around an Acoustically Oscillating Single Air Bubble in Water

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Cavitation microstreaming refers to slow mean flow induced by an oscillating bubble that is subjected to an acoustic field. This type of streaming plays a significant role in microfluidic-based applications where the production, trapping and collapse of a bubble define the performance efficiency of a driving mechanism. In our work, we studied the effect of the water depth on the microstreaming patterns generated around an oscillating bubble attached to a glass coverslip. We used a 3D-printed enclosed chamber with glass coverslips as top and bottom cover to attach and oscillate microbubble with a piezoelectric transducer (PZT). The induced flow patterns depend upon the acoustic energy, bubble size, depth, viscosity and density of the surrounding fluid. We observed that most patterns have some regularity; however, for different water depth the streaming patterns were different.

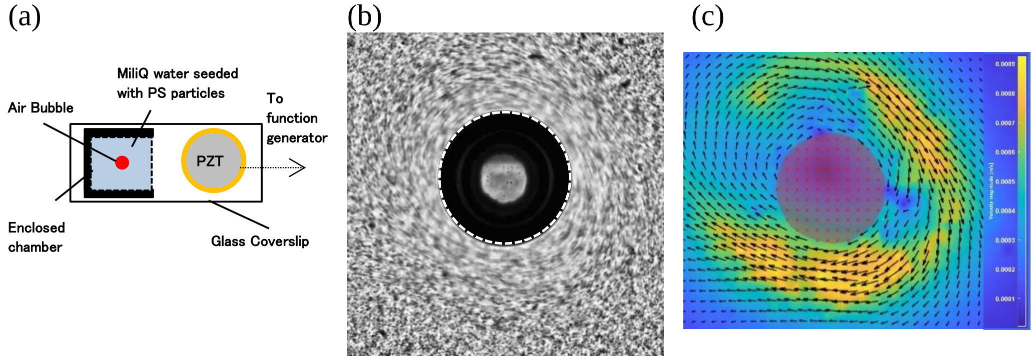

Figure 1: (a) Schematic of bubble oscillation setup, the glass coverslip is mounted on the microscope for observation, (b) an oscillating microbubble showing circular orbiting streaming pattern (dashed circle represents the trapped bubble) and (c) The PIV velocity field (the red circle represents bubble).

Fig 1(b) shows the circular orbiting pattern of a 753 μm diameter oscillating bubble at 2 kHz (20 Vpp) in 2.4 mm chamber. Here, the swirling vortex is seen around the bubble with an eye of the vortex located at a point over the bubble. For 1 kHz (20 Vpp) driving frequency we noted two counter-rotating lobes very close to the interface of 750 μm bubble. The two counter-rotating lobes merged on top of bubble and formed a water jet which pushed the flow away from the bubble. However, the streaming pattern around the bubble was different in a chamber of 1.2 mm in height. Under the same acoustic parameters, the 750 μm bubble had two individual side vortices away from the bubble interface. We argue that the top wall obstructed water flow, and the side lobe pattern morphed into two separate individual vortices.

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Drop breakage using inserts in two-phase systems

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Understanding passive breakage of drops in two phase systems is of crucial importance in industrial applications involving pulsed columns, agitated dispersions etc., Works in literature have majorly focused on breaking drops in air medium with a variety of obstructions [1,2] but seldom mention anything about breaking drops in a two-phase system. We have conducted studies to probe into the outcomes of impingement of buoyant oil drops in water onto wedge shaped obstructions through high-speed imaging. It is observed that a transition from center to off-center impingement can alter the outcome from breakage to no breakage. Similar transition was observed upon decreasing the distance between drop generation and obstruction. It is found that changing the shape of the obstruction has a profound effect with the small-angled wedge breaking the drops easily compared to a wide angled wedge. Another interesting observation was the parent drop breaking and both the daughter droplets leaving on the same side of the obstruction. Experiments to understand the effect of wetting along with generating a phase map to understand how the combination of various forces like buoyancy, drag, wetting, and inertia along with the point of impact affects the outcome of impingements are underway.

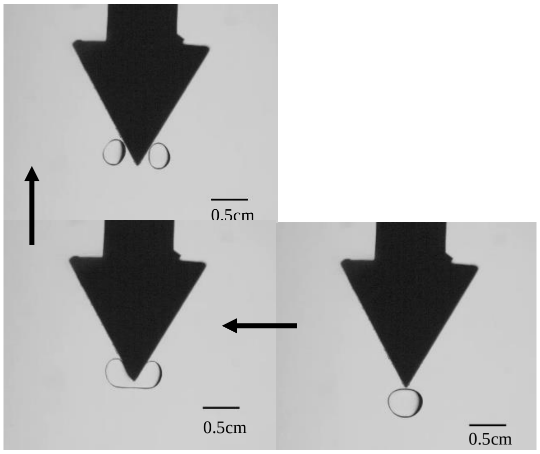

Figure 1: Time sequence for the case of drop breakage

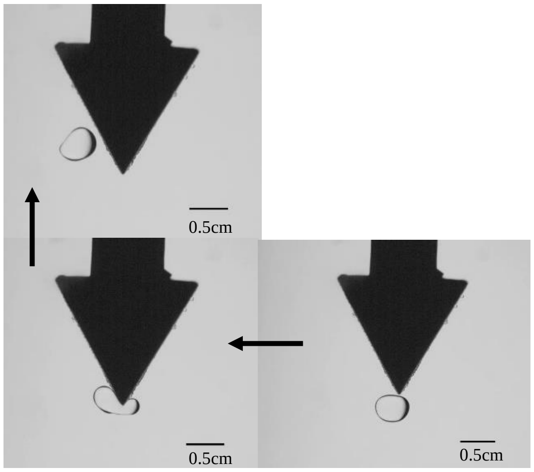

Figure 2: Time sequence for the case of non-breaking off-center impact

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Lightning Stokes Solver for wedge flows: application to moving contact lines

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It is well known that steady Stokes flow in two dimensions can be described in terms of the biharmonic equation for the streamfunction, ψ. In a classical study, Moffatt [1] solved the biharmonic equation and obtained self-similar solutions for wedge flow and found a series of eddies near sharp corners, the so-called *Moffatt eddies*. The biharmonic equation also occurs in elasticity problems where the Airy stress function satisfies the biharmonic equation. Alternative approaches for the biharmonic solution were pioneered by Mushkeshvili [2] using the Goursat representation. The two approaches used in [1] and [2] are shown below:

$$\nabla^4\psi = 0 \implies \begin{cases} \psi(r,\theta) = r^{n+1} f(\theta) \\ \psi(z,\bar{z}) = \mathbb{I}\mathrm{m}\{\bar{z} f(z) + g(z)\} \end{cases}$$

In the first approach, the parameter n is determined by solving a nonlinear eigenvalue problem whereas the second approach involves determining the complex analytic functions $f(z)$ and $g(z)$.

In a series of papers, Trefethen and coworkers [3,4] developed a new technique to solve the biharmonic equation by expanding $f(z)$ and $g(z)$ in terms of rational functions. The new technique is significantly faster than any previously developed technique and is termed as the *'Lightning Stokes solver'*. In this study, we will be using the lightning Stokes solver to first solve for standard problems in Stokes flows and then applying the technique to wedge flows that occur near a moving contact line. A sample result showing the flow field and the distribution of poles near the corners along the resolved corner eddy as shown in figure 1.

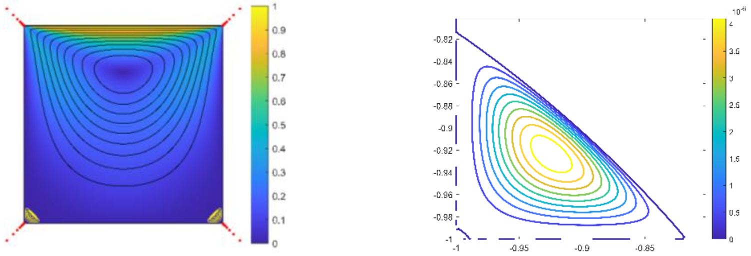

Figure 1: (Left)Contours of stream function in a lid-driven cavity with poles clustered at the corners. (Right) *Moffatt eddies* in the bottom right corner for the same lid-driven cavity flow.

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Modelling the simultaneous entrainment of two liquids with slip

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Dip coating is a technique that has various industrial applications. Modelling the hydrodynamics of dip coating flows is important for understanding how the coating thickness varies with different parameters. In the present work, a mathematical model for simultaneous entrainment of two liquid films from a compound bath containing two immiscible Newtonian liquids [1] has been derived to calculate the thicknesses of the coated films, including the effect of the roughness of the flat substrate [2] by using a Navier slip boundary condition [3], as an extension of the classical Landau Levich problem [4]. The obtained system of coupled ODEs has been solved numerically using COMSOL Multiphysics software using a time dependent formulation. It is interesting to observe that the presence of the outer liquid has a significant effect on the thickness of the inner liquid over a range of Capillary numbers. Though the effect of slip is observed significantly on the thickness of the inner liquid for a wide range of Capillary numbers, it has an effect on the thickness of the outer liquid only for a small range of Capillary numbers, within which, a crossover is obtained that needs to be analyzed in detail.

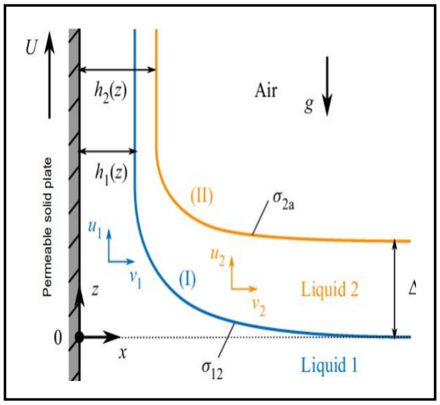

Figure 1: Sketch of the flow configuration described in this work: a permeable substrate is pulled vertically upwards at a constant speed U from a compound bath of two immiscible liquids.

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Development of an electrohydrodynamic solver for polymer electrospinning and analytic modelling of an electrified jet subjected to insoluble surfactants.

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Electrospinning – a technique to produce polymeric non-woven meshes – involves applying a large voltage to a viscoelastic polymer solution emerging through a metal needle. As the voltage increases, electrostatic repulsions overcome the surface tension and the droplet transforms to a Taylor cone. With further increases in voltage, a jet emerges from the cone apex and undergoes a series of instabilities before depositing on a grounded collector. In electrospinning, an interplay between electrostatic force (Maxwell stress) and surface tension force influences the shape of the cone and the jet length which in turn play important roles in determining fiber properties on the collector. It has been shown, for example, that increasing surface tension improves maximum surface charge density and decreases the cone-jet length when the shape transitions from concave to convex [1]. Towards achieving the goal of understanding dynamic changes to cone and jet properties as functions of solution and processing variables, this study involves the development of an in-house electrohydrodynamic DNS solver and a 1D axisymmetric model for an electrified thinning jet. Various OpenFOAM simulations are performed as part of a parametric study in which properties such as surface tension and dielectric constant are systematically varied. To reduce the computational cost, the simulations are carried out on a truncated domain following the procedure outlined by Herrada et al. [2]. The simulations show that increasing the surface tension makes the cone wider and longer, while the converse effect is seen when increasing the dielectric constant, both consistent with previously reported results in the literature [1]. To gain deeper insight, a 1D analytical model is concurrently derived for a thinning electrified viscoelastic jet with insoluble surfactants. These equations are solved numerically using an in-house solver and the results are validated with published literature [3]. Future work will involve direct comparisons with experimental data and stability analysis on an electrified thinning viscoelastic jet with the addition of insoluble surfactants.

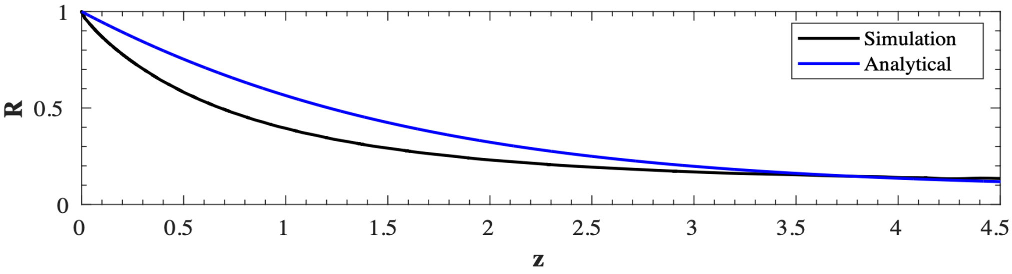

Figure 1: Comparison of radius(R) variation across the axial direction(z) based on OpenFoam simulation and steady-state solution obtained from the analytical model for Glycerol (Radius and axial distance are non-dimensionalised using inner radius of needle)

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Experimental evidence of a slip near a moving contact line

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A moving contact line occurs when the interface between two immiscible phases (Phase A and Phase B) meets a moving solid surface. Conventional boundary conditions such as the no-slip condition on the solid leads to a stress singularity which is sometimes referred to as the moving contact line paradox [1]. Several models have been proposed to relieve the stress singularity and a popular choice is to employ slip at the contact line [2]. In the last decade, new and simpler approaches [3,4] have been developed which allow a region of variable slip near the contact line as shown schematically in figure 1(a). This allows the slip coefficient to continuously vary along the moving wall and the no-slip condition is eventually recovered after a certain distance from the contact line. To date, there is no experimental study which has tested these ideas. Using high resolution PIV, we probe the flow fields near a moving contact line. We plot the total velocity along a curve parallel to the interface as shown schematically in figure 1(b). Interpolating the velocity onto the moving wall, i.e., $r = 0$, we find a distinct jump in the velocity from the moving plate which is interpreted as "effective slip". The radial variation of total velocity for different values of spacing parameter, Δ, is shown in figure 1(c). As Δ increases, the net velocity along the plate, i.e., $|v|_{r=0}$, increases and approach the no-slip velocity of the moving plate. The present study is the first of its kind to conduct a systematic exploration of flow fields in the vicinity of a moving contact line and also contains the first experimental evidence of slip near a moving contact line.

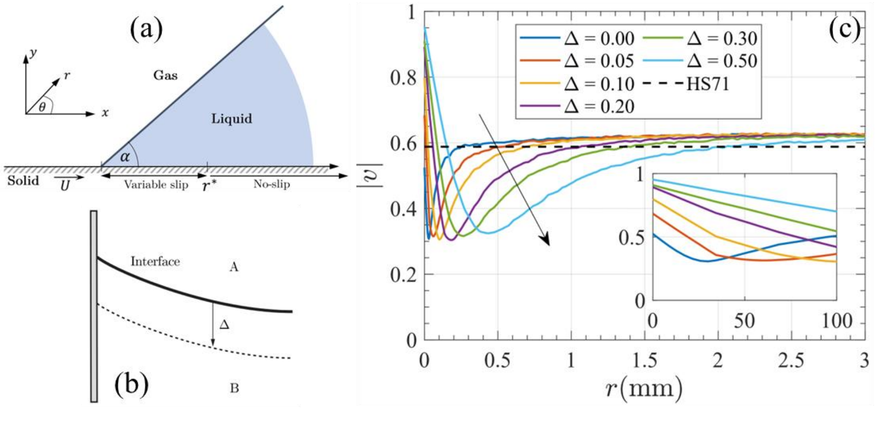

Figure 1: (a) Location where interface shape is extracted in the experiments, (b) Variable slip near a moving contact line, (c) Net velocity along the dashed curves of (a) for different values of Δ.

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Orientation dynamics of a settling spheroid in a simple shear flow

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We have studied the orientation dynamics of a settling spheroid in a simple shear flow. In the Stokesian limit, a spheroid in a simple shear flow exhibits non-uniform periodic rotation orbits. These orbits are known as Jeffery's orbits[1], which is an exact solution in the Stokes regime. The nature of rotation depends on the aspect ratio and initial orientation of the particle. When a spheroid is placed in a quiescent fluid, the orientation of the particle is preserved and indeterminate in the Stokesian regime. The surrounding mean fluid exerts an inertial torque on the settling particle and results in an alignment normal to gravity, hence removing an indeterminacy. Khayat and Cox[2] have used the singular perturbation technique to determine the inertial torque for a high aspect ratio particle. For such a case, a particle's orientation has two fixed points: a stable broadside orientation and an unstable longitudinal orientation. In the current study, we explore the competition of the two torques, shear and inertial, for a spheroid settling in a simple shear flow. The direction of gravity is defined by the Euler angles. The orientation phase space exhibits a rich dynamical behavior that depends on the shape of the particle and the settling parameter. The phase space can have a node-type fixed point where a particle attains an equilibrium angle or exhibits a limit cycle where rotatory motion can occur. The bifurcation diagrams reveal the transition from an oscillating orientation angle to a constant fixed angle predicted by larger inertial torque.

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Theoretical modelling of dark fringe formation during colorimetric detection of Pb using NaRh assay

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The reaction between sodium rhodizonate (NaRh) and lead to form red coloured lead rhodizonate (PbRh), was exploited for the colorimetric detection of lead in water. For ultra-sensitive detection, lead solution was pre-concentrated by homogenous adsorption on kaolin substrate [1]. It is observed that at high concentrations of lead (10-50 ppm), ring-like dark fringes are formed. Thus, it is hypothesised that the porosity of kaolin substrate decreases with an increase in lead concentration. The present study, theoretically analyses the phenomena of spreading and penetration of a liquid droplet on a porous surface for thin and thick substrates. The penetrated liquid undergoes a chemical reaction by adsorbing on porous media coupled with convective mass transport. This study aims to understand the formation of the dark fringes semi-analytically by obtaining the concentration profile of PbRh. This phenomena is modelled by solving the conservation equations of mass, momentum and species by employing the thin film approximation [2]. The equilibrium contact angle is modelled by adopting the concept of a precursor film preceding the droplet contact line. The model is used to investigate the effect of porosity of kaolin substrate on PbRh concentration profile.

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Bag breakup of a polymeric droplet in a continuous flow air stream

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The breakup of a liquid droplet, caused due to the relative velocity with the ambient gas phase (generally air), finds its application in various natural and industrial processes. Such breakup can occur through multiple modes, primarily depending upon the Weber number (We) [1]. However, the bag breakup mode, obtained at low We ($\sim 11-16$), is the most important mode because it demarcates the regime below which there is no further breakup. Hence, this mode decides the minimum fragment size during the air-assisted breakup process. Polymeric droplets (exhibiting viscoelastic properties) are of special interest for two reasons. First, many liquids of practical importance are inherently viscoelastic, and second, polymers can be added as a rheological modifier to control the droplet breakup process.

We present an experimental study on the aerodynamic bag breakup of a polymeric droplet and compare it with the result of a Newtonian droplet. To outline the role of the liquid elasticity, the elasticity number is varied in the range of $\sim 10^{-4}-10^{-2}$ while the Weber number is kept fixed (≈ 12.5). Experiments are performed by allowing a liquid droplet to fall in a horizontal, continuously flowing air stream. It is observed that the initial deformation dynamics of a polymeric droplet is similar to the Newtonian droplet. However, in the later stages, the actual fragmentation of liquid mass is resisted by the presence of polymers. Depending upon the liquid elasticity, fragmentation can be completely inhibited in the timescale of experimental observation (Figure 1). We provide a framework to study this problem, identify the stages where the role of liquid elasticity can be neglected and where it must be considered, and finally, discuss a criterion that governs the occurrence or the absence of fragmentation in a specified time period.

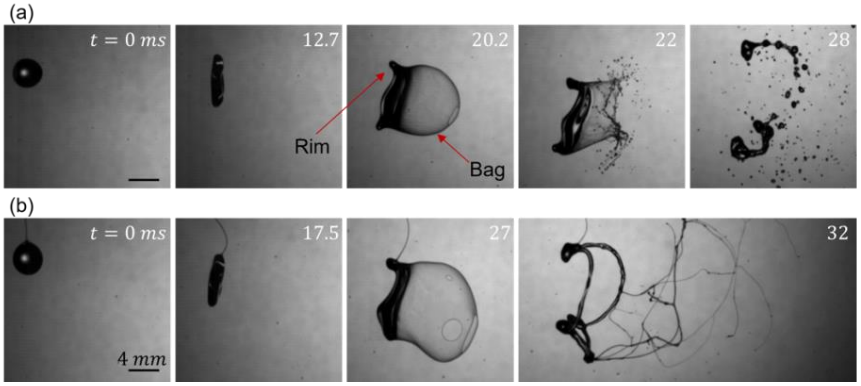

Figure 1: Aerodynamic bag breakup at Weber number ≈12.5 for a (a) Newtonian droplet and (b) polymeric droplet.

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Simulation of Fluid-Particle suspension using the Immersed Boundary Method

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The Immersed Boundary Method (IBM) is a numerical technique for simulating fluid-structure interactions. It handles complex solid-fluid interactions by embedding boundaries in a fluid domain and using interpolation for fluid forces. IBM finds applications in bioengineering, aerospace, and biomechanics, enabling the study of physiological processes, aerodynamics, and biomechanical interactions. With the aim to model such flows, this work proposed to extend the Signed Distance Function Immersed Boundary Method (sdfibm) developed by Chenguang [1], which is bases on OpenFOAM v6. The suggested pyramid decomposition approach and signed distance field representation of the solid shape enable precise calculation of the volume fraction field generated by solids overlapping with a random unstructured fluid mesh. The present work emphasizes on analyses of two-dimensional study of flow past a circular cylinder and three-dimensional simulation of flow past a sphere. The study is done at different Particle Reynolds number between 0.1 and 100. The work is also extended for suspension of particles to analyse the flow between the interstices between particles in the suspension. The Immersed Boundary Method algorithm developed by Shirgaokar [2], implemented in CFDEM opensource simulator is also explored to solve flow around single particle and suspension of particles.

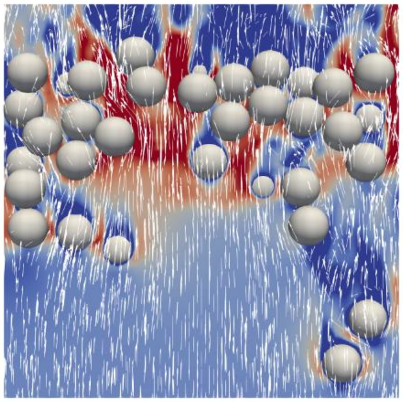

Figure 1: Fluidization of particles

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Stiffness-induced clustering of amphiphilic particles at air-water interface during drying

Vaibhav Raj Singh Parmar*, Sayantan Chanda, Ranjini Bandyopadhyay

The drying droplets of colloidal suspensions are ubiquitous. The kinetics of the drying drop and its final deposition pattern are of great industrial interest. When an aqueous drop of pNIPAM suspension is allowed to dry, the particles migrate to the air-water interface from the bulk due to their amphiphilic nature. We observe a transition from an ordered array of particles at the air-water interface to the formation of clusters when the stiffness of pNIPAM particles is increased. The transition is controlled by the competition between the steric stabilization of pNIPAM particles and their deformability at the air-water interface. When a stiff particle moves to the interface, it changes the air-water interface curvature locally, giving rise to surface tension-originated stress on the particle. As time progresses, these particles experience an attraction toward each other, resulting in the formation of clusters at the air-water interface.

Investigation of spin number and its influence on the cut-size in a spiral air jet mill geometry.

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This work focuses on improving an air jet mill, vital in various industries for finely grinding sub-10 micron powders. Current efficiency is 2-4%, so even minor enhancements could yield substantial energy savings [1]. Notably, spiral air jet mills are gaining prominence due to benefits like no moving parts, low grinding temperatures, and improved maintenance. We start by examining gas flow in the mill using Computational Fluid Dynamics (CFD) and real-world experiments. Spin number, the ratio of tangential to radial velocity, plays a key role. Particles inside experience inward drag and outward centrifugal force. Equilibrium between these forces determines the particle cut size. The equation suggests cut size decreases with higher spin numbers, assuming constant variables. Understanding single-phase flow aids in predicting cut size changes due to particle dilution.

Simulations were carried out for variable gas flow rate (Q), classifier height (ht), classifier radius (rt), rotation (RPM) of the peripheral surface, the chamber sizes (R), the chamber heights (H) of the machine, fluid kinematic viscosity and the machine scale-up. Only one parameter was varied at a time keeping others unchanged from a base case, for univariate analyses. We have found that the spin number decreases with rise in input gas flow rate (Q) and with falling peripheral surface rotation (RPM), increases with higher chamber radial size and lower classifier radius, and spin number is not affected significantly by chamber height and classifier height. As per the simulations carried out in the domain as shown in the figure 1, the machine spin number drops more steeply for higher fluid viscosities. On the experimental front, the runs with different chamber sizes were carried out and it was found that larger diameter chambers yield smaller product particles, the findings of which are in accordance with simulation results (higher spin number yielding smaller product cut sizes). Figure 2 shows the velocity streamlines of the fluid flow from inlet to outlet.

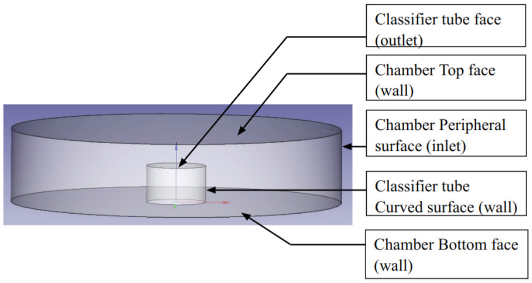

Fig. 2. Schematic of Computational geometry

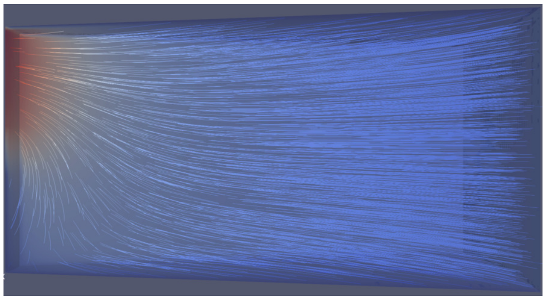

Fig. 2. Velocity streamlines in the front view from inlet (right) to outlet (left).

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Effect of non-spherical drag on particle dynamics in fluidized bed - A CFD approach

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Fluidization process is widely used in chemical, power, pharmaceutical, waste recycling and mineral processing industries. Understanding particle-fluid interactions in fluidized beds is very important for process design and optimization. The Computational Fluid Dynamics (CFD)-based Eulerian-Eulerian approaches have been used to study fluidization process mainly on spherical particles in the past. In the present study, the CFD approach is used to investigate the non-spherical particle dynamics inside the fluidized bed. MFiX-based Two Fluid Model is utilized to study the non-spherical particle dynamics compared to spherical particles. To account for the non-spherical particles used in fluidized bed, different drag models like Gidaspow[1] (1994), Syamlal O'Brien[2] (1989) and Gidaspow-Huilin[3] (2003) are modified by including the sphericity factor from Haider and Levenspiel[4] drag coefficient. The fluidization of spherical and rod-shaped particles are studied and validated against the literature[5]. It is found that modified Syamlal O'Brien model results are closer to experiments. Further, fluidization of the binary particle mixture containing coal and quartz particles with 500 µm in size and 0.8 sphericity in an equal ratio is studied. The segregation rates estimated interms of the mean heights of the coal and quartz particles inside the bed[6] are used to analyze the mixing and segregation of particles inside the bed.

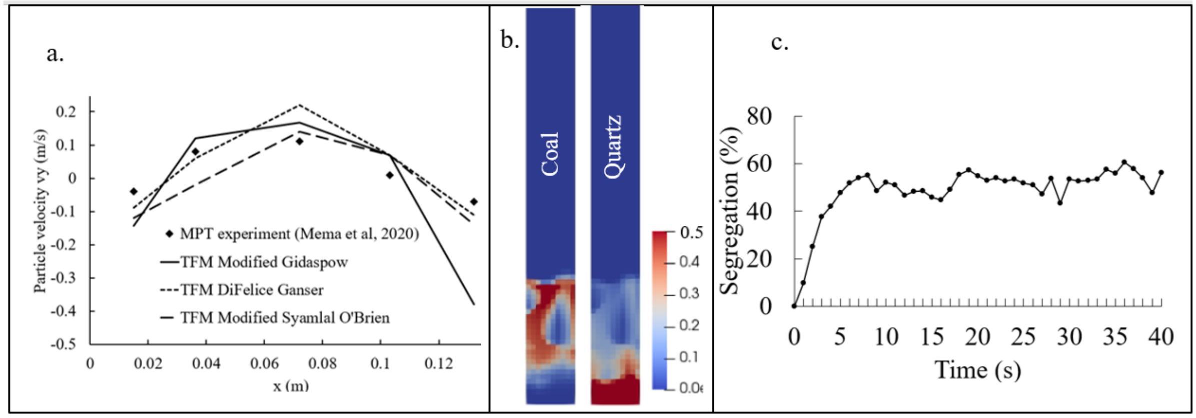

Figure 1: a. Particle velocity profile across the bed during the fluidization of non-spherical particles at superficial gas velocity of 1.6 umf, b. Solids volume fraction during the fluidization of coal and quartz particles and c. Segregation rates with time at superficial gas velocity of 1.4 umf

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Ring formation in the Newtonian rod-climbing effect

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The interface of two immiscible Newtonian liquids, stratified horizontally, exhibits an intriguing counter-intuitive behavior in the presence of a vertically immersed rotating rod. Above a critical rod rotation speed, the liquid-liquid interface shows a climbing behavior near the rod. This phenomenon is referred to as the Newtonian rod-climbing effect. This effect is primarily governed by the viscosity ratio of the lighter to the heavier liquid (μ^*), the rod rotation speed (ω), and the interfacial condition at the liquid-liquid-rod interface [1,2]. For a given combination of liquids, a stable steady-state interface is observed below a certain rod rotation speed (ω_{max}). However, for $\omega > \omega_{max}$, the interface becomes unstable, which leads to the emulsification of heavier liquid into lighter liquid through an intermediate ring-like structure formation, as shown in Figure 1. The instability proceeds as the heavier liquid penetrates continuously into the lighter liquid along the rod surface, leading the heavier liquid to form an annular sheet around the rod (Figure 1 at $t = 4.6\ s$). This annular liquid sheet breaks up to create an emulsion while the topmost portion of the annular sheet develops into a toroidal ring around the rod. Finally, the ring structure breaks up, enhancing the emulsification process. In the present work, we explore the criteria that govern the transition of liquid-liquid interface from a stable to an unstable state and subsequent ring-like structure formation.

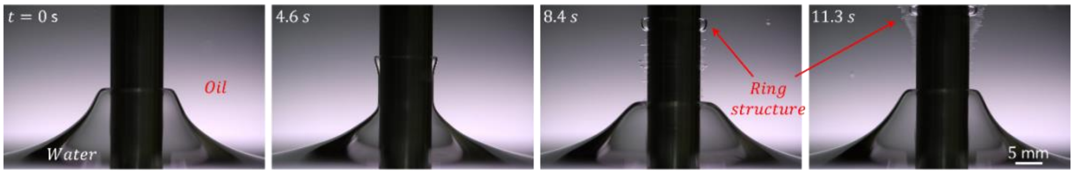

Figure 1: Emulsification and ring-like structure formation in the rod climbing of two immiscible Newtonian liquids for $\mu^* = 355$ and $\omega = 10.8$ Hz [1].

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Surface-directed Spinodal Decomposition on a Chemically Patterned Substrate

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The self-aggregation process in a multicomponent mixture could generate patterns or two- and three-dimensional structures at nano, micro, and mesoscales, with some potential applications in fabricating organic photovoltaics (OPVs) and electronics, photonics, plasmonics, etc. [3,4] The length scales depend upon the mixture's inherent scale; e.g., supramolecular structures formed in phase-separating block copolymers (BCPs) are used to create colors due to their light scattering capability. Self-aggregation is typical of binary fluid mixtures ($A + B$) where the demixing is spontaneous, known as spinodal decomposition (SD) [1], and it is envisaged to generate patterns from nano to meso scales. Moreover, introducing a wall to phase-separating mixtures with preferential attraction to a particular component, say A, causes a wetting layer at the surface due to surface-directed spinodal decomposition (SDSD) [2]. Thin films fabricated over surfaces using spin casting have exploited SDSD to create more efficient OPVs. These OPVs consist of interconnected percolating domains for charges in the photoactive medium and a charge-collecting lateral structure at the electrodes. Such an arrangement has proven to elevate the efficiency of solar cell devices [4].

We extended SDSD by replacing a homogeneous surface with a chemically inhomogeneous one. The replaced surface is now a chessboard where sets of black and white patches are chemically distinct and attract A and B, respectively. In our molecular dynamics (MD) study, the surface registers the pattern quickly in its vicinity compared to patterning due to SD. But the patterns could not survive in fluid layers due to the isotropically growing fluctuations due to SD and are seen to melt in time. We conducted a more elaborate study by quantifying the pattern growth and characterizing the domain morphologies obtained. Conspicuously, we need a better understanding of domain characteristics and their temporal evolution before they can be solidified for desired functionalities.

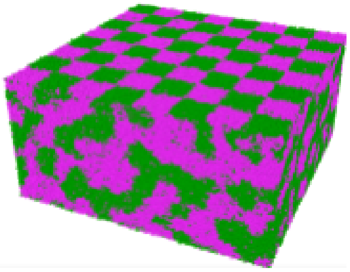

Fig: MD snapshot of a binary mixture undergoing surface-directed spinodal decomposition on a patterned substrate.

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Unexpected differences in the electrohydrodynamic oscillations of charged and polarized anchored water droplets

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Electrostatic manipulation of droplets is one of the popular means to non-invasively manipulate multiphase fluid systems at milli and microscales. The deformation of droplets due to an electric field is an old subject with decades of scientific studies reported in the literature with a variety of fundamental and applied research interests[1]. However, in our high speed imaging experiments we identified, when a water droplet is mechanically held in air in an electric field, its deformation behavior differs qualitatively and substantially depending on whether the droplet is charged or polarized.

When the droplet is held on an electrified metal needle facing an opposite polarity plate electrode, the droplet undergoes transient oscillations before it achieves its deformed shape, due to the influence of electric and interfacial stresses and finite inertia of the liquid droplet. These oscillations dampout quickly with about 10 oscillations. Similarly, when a pair of droplets of slightly different sizes are held on two metal needle electrodes facing each other, the transient oscillations of the droplets fluctuate in amplitude similar to acoustic beats or beating envelopes. These observations are intuitive and inline with the existing theoretical and experimental literature on the electro-deformation of droplets in air.

On the other hand, when the droplet is held on a glass capillary (instead of a metal needle) and placed between a pair of parallel plate electrodes, the droplet is not in direct physical contact with the electric supply and hence not charged but polarized. The resulting electro-deformation oscillations in this case have a similar time period as that of the charged droplet, however, it does not damp quickly but sustains for tens of thousands of oscillations. This behavior is observed above a critical electric field strength and can be explained to arise due to a weak balance between the variation of interfacial tension and the weaker nonlinearity of electric stress with the droplet deformation in the case of a polarized droplet. Similarly, in the case of a pair of polarized droplets, the beating fluctuations were suppressed and their oscillations were always synchronized irrespective of a large difference between the two droplets. These observations not only provoke a fundamental interest in the fluid dynamics aspects of the problem but might as well have significant implications on various applications of electrohydrodynamics.

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Modelling dynamics of an Ultrasound Contrast Agent near a deformable wall using Kelvin Impulse

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Ultrasound contrast agents are microbubbles encapsulated with a shell that is deformable and biocompatible. They are injected directly into an area of interest in the human body and used for vascular imaging, drug delivery and tumor detection. However, issues like allergic reactions and premature collapse of bubble renders UCAs as the lesser used imaging tool. In this study, we use the concept of Kelvin impulse to understand the dynamics of collapse/movement of a UCA close to a deformable wall. We derive the corresponding expression for Kelvin impulse associated to a UCA and track interface deformation using Boundary Integral Method. Deformable effects of the wall are accounted as boundary conditions to potential equation. Interfacial dynamics and bubble motion is captured to understand the radius/distance from wall threshold at which bubble collapse occurs.

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Improved surface tension force scheme for two-phase flow in diffuse interface framework

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In the diffuse interface models, the surface tension force is smoothly localized around the interface region. We look at Laplace pressure error in the case of a drop suspended in another fluid at the steady state. Here, errors in pressure can be expressed in terms of two small parameters- one relating to the grid resolution and the other to the Cahn number. We use Allen-Cahn equation for interface tracking in the diffuse interface framework. We find that the small parameter related to grid resolution has a larger effect on the surface tension error than the Cahn number. This observation is justified by expanding the phase-field variable in terms of grid resolution in the interface tracking equation. The deviations of the phase field from its equilibrium are then used to estimate the error in the momentum balance equation. The non-equilibrium part of the surface tension force was found to explain the error in the Laplace pressure to a large extent. Based on this, we suggest a correction to the numerical surface tension that significantly reduces the errors as shown in Figure 1. The Lattice Boltzmann method was used for numerical validations, although the findings are applicable to any methods using regular grids.

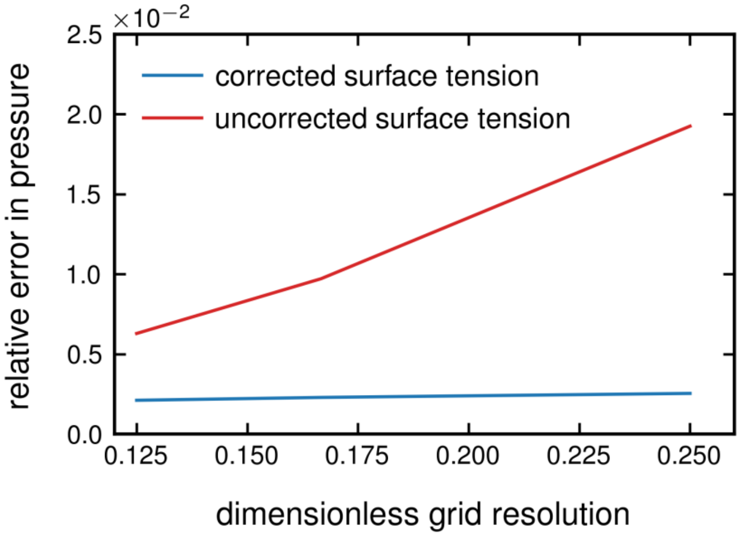

Figure 1: Relative error in pressure with decreasing grid resolution for both uncorrected and corrected surface tension. For corrected surface tension the errors are significantly lesser.

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Entrapment of air-borne particles by pulmonary mucus films

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The air we inhale brings along with it a variety of aerosol particles---dust, pollen, bacteria, and viruses---which can damage the inner wall of the tubular airways and lead to infection [1]. The primary defense against such air-borne particles is the thin film of mucus that lines the inner wall of the airway [2]. While several studies have simulated particle transport in the lungs, they have typically ignored the interfacial dynamics of the mucus film. In this work, we consider a single pulmonary airway, and ask whether the well-known Rayleigh-Plateau instability, which produces a non-uniform film thickness with bulges of mucus interspersed with dried-out regions (Fig. 1a), aids or inhibits particle entrapment. We develop a long-wave model that considers (i) the coupled fluid dynamics—in small-inertia and long-wave limit [3]—of the air and mucus phases, (ii) the deformation of the air-mucus interface induced by capillary forces, and (iii) the transport of mucus by a carpet of synchronously-beating cilia. The motion of particles is treated by solving the Maxey-Riley equation for inertial particles, augmented by Brownian forces. Using this model, we determine the relative fractions of particles that are trapped by the mucus and that deposit on the dried-out portions of the airway wall.

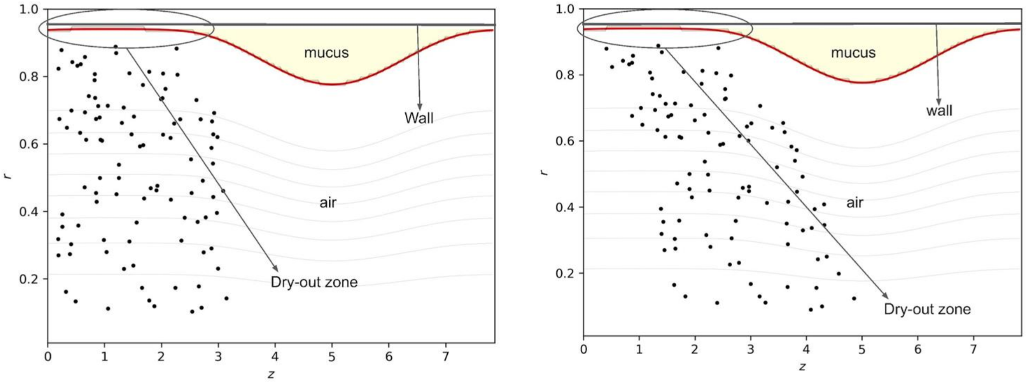

Figure 1: Snapshot of a simulation of airborne-particles transported past a deforming mucus film

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Extensional rheology of polymer solutions for spray application

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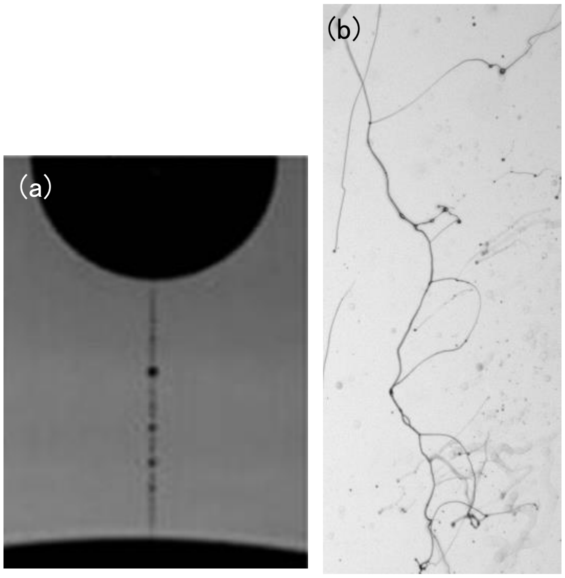
Polymers are widely used in industries like agriculture, pharmaceutical, spray painting, etc. The breakup of polymer jets into droplets by undergoing primary atomization, followed by secondary atomization into satellite droplets, plays a pivotal role in these applications.

The present study focuses on the effect of the extensional relaxation time of polymer on the jet breakup phenomena. Xanthan gum (XG), an anionic polysaccharide with M_w= 2.7 MDa, is used for the experiment. Different concentrations (0.1,0.5,1.0) % wt. XG are used to observe the atomization of polymer solutions using a rotary atomizer. All solutions exhibit a Newtonian plateau followed by strong shear thinning behavior with increasing shear rates. The CaBER-DoS method is used to determine the extensional relaxation times of all XG solutions.



(a) CaBer–DoS used for assessing pinch–off dynamics of 0.05% PEO[1].
(b) Bead–on–a–string(BOAS) structures formed during the breakup process of 1% XG.

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PH-O1

Self-Assembly in Block Copolymer/Nanoparticle Mixtures

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The self-assembly of block copolymers (BCP) has been an area of intense investigation for more than two decades now. The interest in these polymers lies primarily because of their ability to self-assemble into various periodic nanostructures depending on the BCP composition and block ratios. The ordered nanoscale morphologies formed by the block copolymers and the chemically distinct nature of the blocks constituting the copolymer allow them to be used as templates to host and direct the assembly of externally added additives such as inorganic nanoparticles (NP). A number of studies, both theoretical and experimental, have been done in this direction, with a focus on controlled localization of nanoparticles in the microphase separated structure of block copolymers. Here, some of the work being done in our group, in this direction, will be discussed [1-4]. It will be shown that the block copolymer/nanoparticle mixture may result in the formation of interesting and unexpected morphologies and hierarchical structures. Furthermore, it will also be demonstrated that these bulk hybrid materials may further be suitably treated to isolate individual nano-objects with well-defined shape.

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A Multifaceted Transesterification Route to Functional Polyesters

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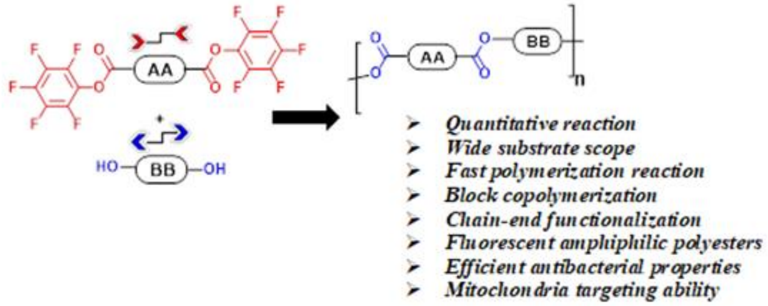
Abstract: We have demonstrated a versatile and effective condensation polymerization method for the production of functional aliphatic polyesters (Figure 1).[1] A vast library of polyesters with a degradable backbone can be generated through organo-catalyzed (4-dimethylaminopyridine) transesterification[2] reactions between an activated pentafluoro phenyl-diester of adipic acid and structurally different diols ranging from simple linear and cyclic to quarternized naphthalene monoimide (NMI) moieties. This approach, with the help of a "monofunctional impurity" or "stoichiometric imbalance," is capable of producing well-defined end-functionalized polyesters with predictable molecular weights and narrow dispersity under mild reaction conditions. The less nucleophilic pentafluorophenol released as a byproduct requires no removal, allowing the polymerization reaction to proceed rapidly. This has been a significant issue in traditional polyester synthesis using non-activated diesters. The polymerization kinetics evaluated in the presence and absence of the catalyst revealed significant changes in conversion rates, suggesting that the catalyst plays an important role in the polymerization reaction. Block copolymer synthesis by chain extension following either controlled radical polymerization or ring-opening polymerization has also been successfully accomplished. Following this methodology, positively charged, fluorescent aromatic dyes could be introduced as pendants in the polyester backbone. These enzymatically degradable, water-soluble polyesters exhibit great potential as broad-spectrum antibacterial agents. The antibacterial properties of these polyesters could be tuned by varying the molecular weights and/or incorporating long alkyl chains within the aromatic pendant. These fluorescent amphiphilic polyesters produce stable micelle-like aggregates in water and display potential mitochondria targeting ability through efficient cellular absorption via the endocytosis pathway.



- *Quantitative reaction*
- *Wide substrate scope*
- *Fast polymerization reaction*
- *Block copolymerization*
- *Chain-end functionalization*
- *Fluorescent amphiphilic polyesters*
- *Efficient antibacterial properties*
- *Mitochondria targeting ability*

Figure 1. *A generally applicable synthetic scheme for functional polyesters by a transesterification method using an activated diester monomer.*

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Intrinsic Viscosity and Rheology of Ring Polymers

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Abstract

A ring polymer is formed by joining the free ends of a linear polymer. The interest in ring polymers is motivated by the biological relevance of its cyclic architecture. Many biopolymers such as DNA, lipids, polysaccharides, and polypeptides exist in nature as rings. Ring polymers in different solution conditions may be an excellent model system for exploring the properties, interactions, packing and specific fonctions of these circular biomolecules. The conformational properties, rheology and segmental relaxation dynamics of ring polymers are investigated within the framework of optimized Rouse-Zimm theory. Smaller rings relax faster than larger rings and their respective linear analogues. The hydrodynamic interactions decrease the higher relaxation rates corresponding to the local relaxation modes and increase the smaller relaxation rates, which correspond to the collective relaxation modes. The structural properties, like the mean square radius of gyration, static structure factor, scattering intensity, the fractal dimensions, and the mean square intermonomer distances of ring polymers in are calculated in dilute solutions with excluded volume interactions, where the strength of these interactions are evaluated from Flory's mean-field theory. The mechanical moduli are dominated by the smaller relaxation rates corresponding to the collective relaxation modes in the low frequency regime, while they are governed by the higher relaxation rates. The characteristic overall relaxation time is found to be same for the rings of various sizes with excluded volume interactions, whereas it shifts to lower frequencies with increasing ring sizes for the Rouse rings.

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PH-O4

Solvation Shell Thermodynamics of Extended Hydrophobic Solutes

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Interfacial solvent density fluctuations play an important role in hydrophobic effects, which regulate the functional characteristics of a wide variety of soft matter system [1]. The inability of water molecules to maintain their hydrogen bonded network around extended interfaces leads to enhanced density fluctuations near large non-polar solutes, which make their hydration shells susceptible to small perturbations [1]. Cosolutes can either enhance or quench the interfacial solvent density fluctuations and thereby regulate the hydration behavior of non-polar solutes, which results from their preferential accumulation or depletion on the solute surface [2,3].

To understand the molecular mechanisms and driving factors behind these observations, we employ atomistic computer simulation to investigate the solvation behavior of molecular solutes. We investigate the effect of two adsorbing cosolutes: urea and methanol on the interfacial density fluctuations of a model extended hydrophobic solute. We found preferential accumulation of urea to quench the density fluctuations around the extended solute, leading to a decrease in the compressibility of the solvation shell. In contrast, methanol accumulation enhances the density fluctuations, leading to an increase in the compressibility [3]. To isolate the dominant interactions that lead to these contrasting effects, we also explored the energetics of the solute solvation shells. Our results showed that the effect of these adsorbing cosolutes on the solvent density fluctuations, and thereby the stability of the solvation shell, is strongly coupled to their hydration behavior. The observations from this simple model can be discussed in the context of cosolute induced swelling and collapse of polymers in aqueous solutions.

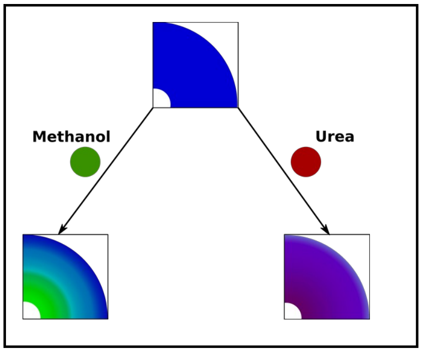

Figure 1: Schematic showing the distribution of water and two preferentially accumulated cosolutes, methanol and urea, in the solvation shell of a model extended hydrophobic solute. Methanol and water molecules are segregated whereas urea and water molecules are more uniformly distributed.

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PH-O5

Development of Conducting Polymer Nanocomposites for Energy Harvesting Applications

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Conducting polymers are usually good candidates for electrode materials of supercapacitors in spite of their lower cyclic stability, which can further be improved by combining with suitable nanofillers. We have explored a wide range of nanofillers with polyaniline (PANI) as the conducting polymer. Some of the nanofillers are caron-based, such as graphene, graphene oxide, reduced graphene oxide. The other class of nanofillers are metal oxides, such as MnO_2, MoS_2 and ZnO. We have shown that an appropriate proportion of the nano fillers with PANI enhances the supercapacitance performance. We have also explored the combination of more than one nanofilers from different types, for example, graphene and MoS_2, graphene and MnO_2, reduced graphene oxide with ZnO, etc. We have followed in-situ polymerization to synthesis PANI from aniline, ensuring the formation well-dispersed nanocomposites. Detailed structural characetrization shows the uniform distribution of nanofillers within the PANI matrix. Electrochecmical characterization shows that the supercapacitance performance has been enhanced significantly in the presence of nanofillers. In this presentation, some of the systems that we have studied recently, will be discussed.

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PH-O6

Universality of dilute ring polymer solutions

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The unique behaviour of ring polymers solutions is believed to arise from their peculiar topology of having no chain ends. There have been many studies aimed at obtaining a thorough understanding of the physics of ring polymers, and amongst the key properties that have been examined are their size and dynamics, which are distinct from their linear chain counterparts. In the case of linear homopolymers of high molecular weight, it is well known that various static and dynamic properties of dilute solutions exhibit universal behaviour, with data collapsing onto master curves when represented in terms of suitable scaling variables. In contrast, however, studies examining the universal behaviour of dilute ring polymer solutions have been relatively sparse. In particular, to our knowledge, there have been no experimental or computational studies that have systematically examined the existence of universality in ring polymer solutions in the intermediate regime between θ and athermal solvents. In this talk, we present the results of our recent study, using Brownian dynamics simulations, of the universal thermal crossover behaviour of dilute ring polymer solutions. We find that there is a fundamental difference in the scaling of static and dynamic properties of rings and linear chains in this regime, which requires validation through careful experiments. While the current work is focused on understanding static and dynamic equilibrium behaviour, this knowledge is essential even away from equilibrium in order to develop simulation models of flowing solutions that replicate their solvent quality in the thermal crossover regime.

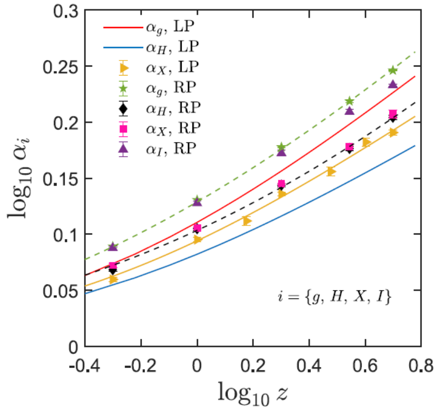

Figure 1: Swelling ratios plotted as a function of solvent quality, z, for linear (LP) and ring (RP) polymers.

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MORPHOLOGICAL CONTROL DURING POLYMER CRYSTALLIZATION

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Semicrystalline polymers play a vital role in many applications, from food and beverage packaging to strategic materials in military applications. The semi-crystalline morphology controls many key properties (e.g. barrier and mechanical properties) making precise control of keen interest. We review recent and ongoing work towards this end along two lines (i) directional solidification of melts and (ii) morphological instabilities during melt solidification. For both, we have pursued minimal continuum-level modeling consistent with essential physics. 1-d directional solidification models for a melt just above the melting point by a moving heat sink clarify the essential physics of this process. The minimal models include heat dispersion, latent heat release, and autonomous crystallization kinetics (either Avrami-like or interfacially nucleated crystallization). In either case, for realistic parameter assignments, melt crystallization is confined to a narrow (boundary) layer near the solid-melt interface. The models make clear the basis for the anzatz of Gryte and Lovinger of an equivalent undercooling for directional solidification scaling with the sink speed, as well as the existence of an upper bound on the sink speed. We also consider from the same continuum models the spontaneous development of frond-like morphological instabilities during the solidification of an undercooled, metastable melt, controlled by thermal gradients (Mullins-Sekerka instability) using a unique numerical algorithm.

Collapse transition in a model heteropolymer: Effect of chain topology

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The collapse transition of an energy polydisperse chain, a model heteropolymer chain where the number of monomer species is same as the total number of monomers, is studied using molecular dynamics simulations. Each monomer is assigned an interaction energy drawn randomly from a Gaussian distribution and disparity in the interaction values is characterized through polydispersity index. In this study, the effect of chain topology on the collapse transition and instantaneous shape are being investigated. Three different chain topologies, namely, linear, ring, and trefoil knot are considered. A particular question of interest that we address is whether the chain topology and energy polydispersity affect the nature of two-stage transition, i.e., extended coil to globule followed by globule to freezing at sufficiently low temperature.

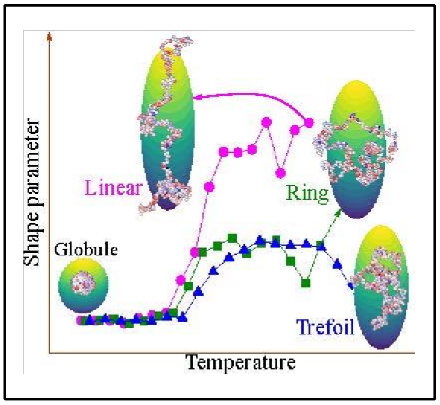

Figure 1: Difference in the shape of three topologically different energy polydisperse chains at different values of temperature.

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Plant-inspired Mechanosensitive Soft Robots

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Modern society relies on robotic automation to accomplish menial, hazardous, and sophisticated tasks. A growing subfield of robotics uses soft materials to accomplish these tasks. While promising, soft robots typically lack a key feature: mechanosensitivity. To address this challenge, we designed a smart skin transmitting information using non-linear poroelasticity in a fashion reminiscent of plant mechanoperception. More specifically, we used a strain-softening material, Ecoflex©, to design a skin perforated with channels filled with a liquid that we implemented on a homemade 3D-printed arm and connected to a pressure sensor. When the robot arm grasps an object, the skin deformation leads to a superlinear increase in pressure, enabling accurate stress measurements. We could then access experimentally the strain applied by the robotic arm and use these inputs in combination with contact mechanics theory to extract the radius and effective Young's modulus of the grabbed object. As such, this innovative skin broadens horizons for automation, equipping robots with the capability to assess soft object stiffness and ensuring safer interactions with humans.

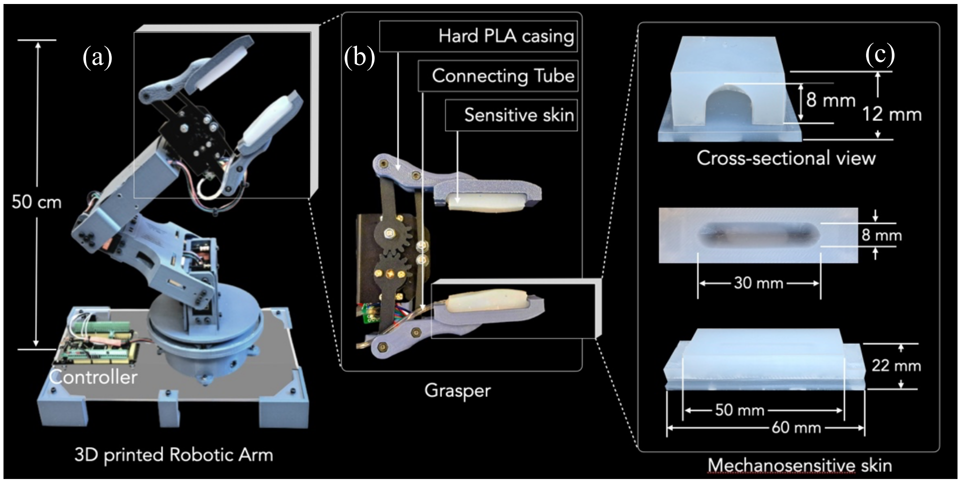

Figure 1: Plant-Inspired Soft Robot (a) Homemade 3D-printed robot with feedback control system. (b) Magnified view of the grasper, featuring a hard PLA casing embedded with strain-softening Ecoflex© skin. (c) Magnified view of the strain-softening skin, showing its dimensions, internal channel structure, and cross-sectional view of the channel.

References

1. NA

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Local Drug Delivery to Pancreatic Tumor by Film and Gel-based Polymeric Implants

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Pancreatic cancer is one of the most difficult to treat among all cancer types and the survival rate has not improved over last many decades. So, there is an unmet need to develop better ways for delivering anticancer drugs to pancreatic cancer patients. Gemcitabine (GEM) is a stand-alone chemotherapeutic drug reported to increase the survival of pancreatic cancer (PC) patients. However, main challenges in systemic injection of GEM have been: (i) Its inability to reach PC cells because of dense stroma, (ii) its low plasma half-life and low bioavailability and (iii) its cytotoxicity to healthy cells and development of resistance to PC cells. This necessitates a continuous, pre-determined, slow and controlled release profile of the drug near the tumour tissue. This has been achieved by us, on developing drug-loaded polymeric implants, rather than a burst release seen in conventional drug carriers.

To this end, we have formulated and performed pre-clinical animal trials of both film (Figure 1) and gel-based polymeric implants, containing GEM. GEM being highly hydrophilic, we used chitosan for developing the film or gel. Furthermore, we combined polyvinyl alcohol (PVA) with chitosan, which reduced the elastic modulus and increased the mechanical strength. The film was crosslinked, to achieve a favoured cross-sectional, drug-concentration profile, leading to slow release of GEM over weeks. When GEM is delivered by film, it has enhanced cell-killing capability in 2D and 3D cell models. Also, GEM-film showed prominent cytotoxic effect on GEM-resistant cells and did not lead to development of GEM-resistance, unlike free GEM. In the orthotopic mouse PC model, GEM-film significantly regressed tumour growth in comparison to free GEM-treated group, without use of implant.

Recent studies have also shown that, curcumin (CUR) can potentiate the anticancer effect of GEM. So, in line with the film, we have combined CUR with GEM, to develop a chitosan-PVA composite gel of dual drugs. The gel displays a desirable, controlled release of both the drugs in acidic pH (pH of pancreatic tumour microenvironment is 5.5). On optimizing rheological and functional properties of the gel, it also displayed higher anti-tumour efficacy and reduced cell proliferation, compared to free drug, in orthotopic mouse models.

In conclusion, controlled, local release of drug from an implant near a tumour, has enhanced cytotoxicity on PC cells and higher mouse survival. Hence, we propose, implants may be used for local delivery of drugs in PC patients. Our current work on engineered film and gel implants, via lab-on-a-chip systems, aims to elucidate the link between film and gelmicrostructure to drug transport and its efficacy, before possible future clinical trials .

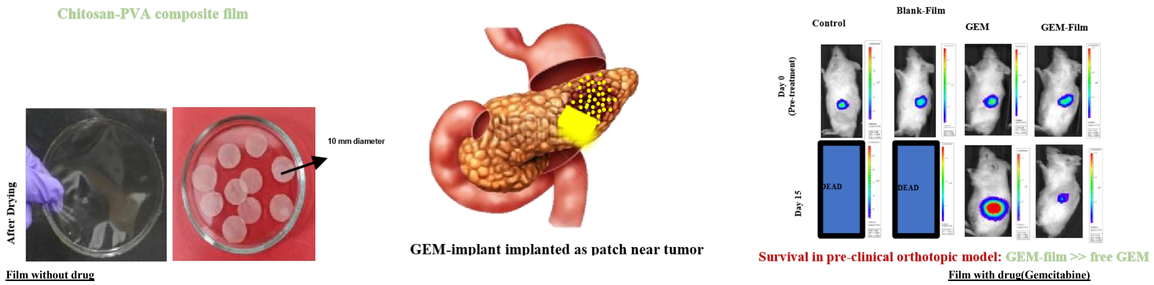

Figure 1: Drug delivery by polymeric implant for tumour regression and higher survival

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Polymer complexation: Theory and application to the thermodynamics of complexation between highly charged disordered proteins

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We present an analytical polymer model of polyelectrolyte complexation (PEC)[1,2], based on the Edwards-Muthukumar Hamiltonian[3,4] and counterion condensation and release[1,2], to quantitatively describe the driving forces of interaction of the ProTα- H1 complexation. This model of PEC takes into account conformational properties of the individual IDPs, counterions associated to the IDPs, and the free salt ions, resulting in several free energy contributions of enthalpic and entropic origin. Free volume entropy of the condensed and released counterions, Coulomb energy of the bound ion-pairs - both of the counterion-protein and protein-protein types, and electrostatic correlations of free charges are found to contribute most significantly to the thermodynamics, whereas the excluded volume or site-specific interactions seem overwhelmed by electrostatic interactions. The dielectric mismatch between the bulk solvent and regions close to the proteins plays a crucial role in the energetics of the complexation. The model captures the thermodynamics of protein complexation, both in terms of the reaction enthalpy and free energy for different salt concentrations, as well as the salt concentration dependent chain dimensions, with only four adjustable parameters[5]. The model quantitatively matches with the experimental finding[5] that the entropy gain from the released counterions is the primary thermodynamic driving force of the complexation, whereas an enthalpy loss opposes the process.

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Simulation of PE Hydrogels with complex network topologies

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TThe Polyelectrolyte hydrogels have a unique ability to act as desalinating agents when placed in a salt solution and they exhibit a high absorbency exceeding several times their own weight. In the more recent experimental studies, hydrogels have been applied to desalinate salt water in a membrane-free forward osmosis process[1] and the charges inside the polymer lead to unequal distribution of salt between gel and solution phase and hence increased concentration of salt in the supernatant. Homogenous network structures can be easily prepared in the lab[2] and they are studied extensively through theoretical models and computer simulation[3]. We want to investigate the effect of network heterogeneity on macroscopic quantities such as swelling capacity, mechanical properties and salt partition. Polydispersity in the chain length was added in the mean-field gel models[4,5] and swelling results showed pronounced differences when compared to simulation which takes explicit polydispersity[6] and further work is needed to understand this mismatch better. For superabosrbers, it is desirable to have increased swelling capacity without compromising the bulk modulus. To this end various network structures will be designed and studied such as hydrogels with dangling ends, dendrimers, charged inclusion of polyelectrolyte stars and also modifying polyelectrolyte backbone to consist of bottle-brushes. These structures allow realising high charge density without significantly increasing the bulk modulus. In the simulation, the gel would be imposed with different volumes to obtain a PV curve which allows us to calculate the Isothermal bulk modulus when the system is in equilibrium with the ionic reservoir. Further, we also plan to study the effect of multivalent ions by enhancing the previous coarse-grained models[7,8] to include ion specificity. Our goal is to reach a quantitative understanding of the difference certain ionic species can have on salt partitioning, swelling behaviour as well as on mechanical strength. For this purpose, we also augment the PB model with Lennard-Jones potential whose energetic depth can be fitted with all-atom results[9,10] and its solution can be compared with the simulated ionic distribution. We also want to study the relaxation of gels with different degrees of crosslinking and network topology by recording the position of each monomer and implementing an algorithm to calculate the autocorrelation function. The simulated results can be verified by experimentally obtained T2 relaxation rates[11]. We also plan to improve the osmotic engine by finding the best parameters for the highest power production through the help of simulation.

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PH-P1

Nanoclay based hierarchical mesoporous polyaniline/acetylene black nanocomposites for high energy density supercapacitors

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Investigating new electrode materials is one of the most important steps in creating high performance energy storage systems to effectively utilize renewable energy. Clay minerals, notably montmorillonite (MMT), could be a possible candidate for electrode materials due to their naturally porous structure, strong ionic conductivity, high specific surface area, and environmental friendliness. However, due to their poor electrical conductivity, MMT cannot be used as a sole electrode material for supercapacitors. Therefore, to change the surface conductivity, conducting polymers would be a good choice. In this study, we have developed a novel ternary nanocomposite by in-situ chemical oxidative polymerization employing polyaniline (PANI) as the conducting polymer, acetylene black (AB), and MMT with varying mass ratios. The electrochemical performance of all the composites as electrode material for supercapacitors were examined. Among all the other synthesized nanocomposites, the ternary composite PANI/AB/MMT (16:1:1) displayed the highest specific capacitance and excellent cyclic stability. Further investigation has been done on the constructed symmetric capacitor based on the PANI/AB/MMT (16:1:1) nanocomposite in both aqueous and solid polymer electrolytes (viz., PVA/H_2SO_4). In the solid electrolyte, the device generates specific capacitance of 772 F/g, energy density of 107.2 Wh/kg, and power density of 2000 W/kg at a current density of 1 A/g. Moreover, after 6000 cycles at a current density of 5 A/g, the device shows the capacity retention of ~ 98%. The increased performance of electrode material is attributed to the synergistic interaction of the three components, which results in an improved electroactive sites, increased surface area, mesoporous structure, reduced internal resistance, and high chemical stability.

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PH-P3

Structure-Property of Epoxy Blends in Electronic Packaging: Impact of Heating Rate

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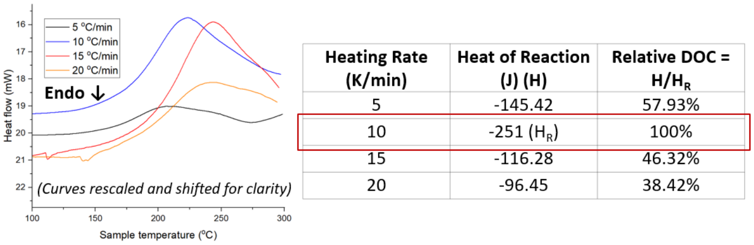
Epoxies are extensively used in semiconductor packaging as prepreg resins in copper clad laminates, underfills in flip-chips, encapsulants and dielectric layers in high density interconnect (HDI) substrates. Here, we investigate structure-property relations in blends of epoxies, rather than their composites, as such blends have not been investigated in detail in relevance to advanced electronic packaging. Specifically, the effect of heating rate during curing is being explored on parameters that are relevant to electronic packaging. A few such parameters are peak curing temperature, glass transition temperature (T_g), dynamics of curing, degree of cure and water absorption behaviour of the network. The microstructure of the network is dependent on the curing rate and controls the T_g [1]–[3] and water uptake behaviour [4], [5] of the blend.

In this study, a blend of diglycidyl ether of bisphenol-A (DGEBA) and a multifunctional epoxy were cured at various heating rates using an amine hardener. The reaction mechanism consists of two steps [6]: (i) conversion of primary amines to secondary amines, leading to the formation of long, linear chains and (ii) conversion of secondary amines to tertiary amines, leading to cross-linked network formation. FTIR analyses show the conversion of epoxides to hydroxyls and primary amines into secondary amines. The dynamics of the curing behaviour were studied using DSC. The relative degree of cure (DOC) and T_g increased with heating rates, showing a maximum when heated at a rate of 10 K/min, after which they decreased. The relative DOC was calculated by the ratio of the heat of curing at a given heating rate (H) to the maximum heat of curing (H_R) which, in this case, was for the blend cured at 10 K/min.



Heating Rate (K/min)	Heat of Reaction (J) (H)	Relative DOC = H/H_R
5	-145.42	57.93%
10	-251 (H_R)	100%
15	-116.28	46.32%
20	-96.45	38.42%

Figure 1: DSC curves showing curing peaks for blends cured at different heating rates from 5 to 20 K/ min.

The increase and subsequent decrease in these properties imply that the nature of the cross-linked network is controlled by reaction time, reaction temperatures and reaction mechanism. At lower heating rates the conversion of primary amines into secondary amines is favoured due to their higher reactivity, leading to a network with long polymer chains with very few cross-links. Higher heating rates allow secondary amines to be converted to tertiary amines, forming networks with higher cross-link densities. However, if the heating rate is too high, the reaction may not have enough time to complete. This results in an incompletely cured network with a low cross-link density filled with monomers that act as plasticizers leading to reduced T_g. The blend cured at the optimal rate of 10 K/min had a T_g of ~210 °C, which fulfills one of the requirements for dielectrics as per Semiconductor Research Corporation [7].

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Diffusion of star polymers in dilute solutions: role of shape anisotropy

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Polymer chains dissolved in a solvent take a multitude of conformations due to large internal degrees of freedom and are characterized geometrically by their average shape and size. The radius of gyration (R_g) represents the size of the polymer chain. The diffusion dynamics of polymer chains is one of the most widely studied problems in polymer physics. It is useful in drug/protein delivery and understanding the transport of molecules containing plasmids and amino acid derivatives. The influence of the size of the polymer chain on its diffusion is well studied and best described by Zimm theory with intra-chain hydrodynamic interactions, which predicts $D \sim R_g^{-1}$, where D is the translational diffusion coefficient. However, the influence of the shape of the polymer chain on its diffusion has been studied scantily. In the present work, we are taking a unique approach to understanding the classical problem of diffusion dynamics of the polymer chains in terms of their shape parameter: relative shape anisotropy (κ^2) using a mesoscopic coarse-grained simulation technique, namely Multi-particle Collision Dynamics [1]. Star-shaped chains of varying degrees of functionality (f) are modeled in a good solvent in the limit of infinite dilution. The radius of gyration of the star-shaped chains scales with the chain length (N) as: $R_g \sim N^{\nu}$, with a functionality independent exponent, $\nu \sim 0.627$. We note that highly anisotropic star-shaped polymer chains have a faster rate of diffusion along the translational direction due to a slower rate of rotational diffusion when the radius of gyration of the polymer chains is maintained constant [2].

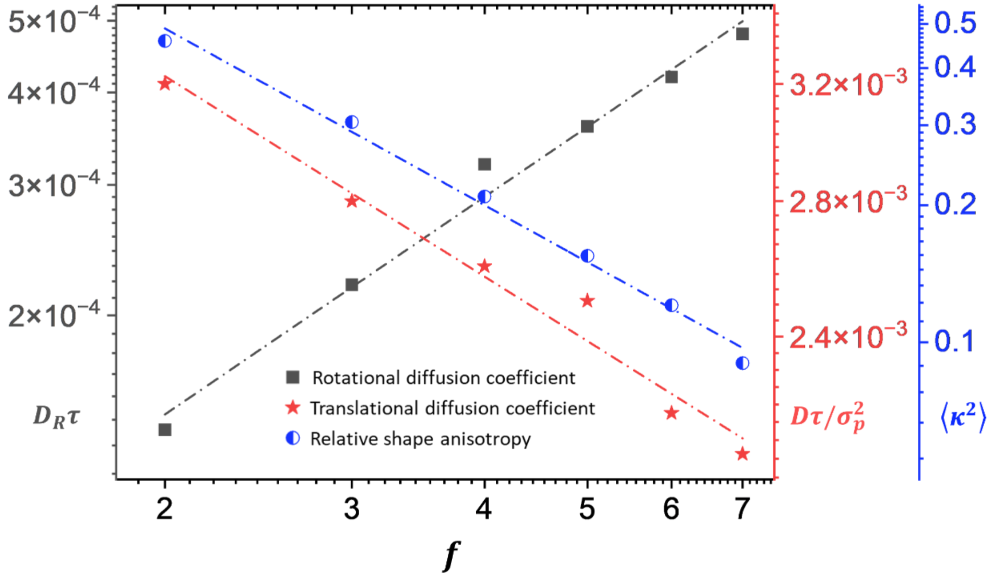

Figure 1: Variation of relative shape anisotropy (κ^2), translational diffusion coefficient (D), and rotational diffusion coefficient (D_R) with functionality (f) of the star polymers with the same value of R_g. Dashed lines represent power law fit. σ_p is the diameter of a monomer bead and τ is the Lennard-Jones unit of time.

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PH-P5

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Phase separation kinetics of miktoarm star polymer in solvent: A DPD simulation study

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ABSTRACT

We present dissipative particle dynamics (DPD) simulation results of a phase-separating polymeric solution in d = 3[1, 2]. The solution contains miktoarm star polymers (MSP) consisting of six alternate incompatible polymer chains, denoted as A_n and B_n , which are covalently connected to a central bead C. The initially homogeneous polymeric solution is prepared at a high temperature and subsequently quenched to a lower temperature, causing the system to become thermodynamically unstable and undergo phase separation into its components. The segregation phenomenon is studied by varying the chain length, L_P. For smaller chain lengths, we observe no segregation. However, at higher chain lengths, segregation occurs due to the competition between enthalpy and entropy of the system. The characterization of the morphology of the segregated system is performed using radial distribution functions, correlation functions, structure factors, and growth laws. The domain size follows a power law relationship: $R(t) \sim t^{\varphi}$, where the dynamic growth exponent is denoted as φ[3].

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On the structure-viscoelasticity relationship of reversible polymer networks

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Reversible polymer networks (RPNs) have widespread applications in self-healing materials and recyclable plastics. [1] These polymeric materials embody functional groups which can be programmed to form irreversible or reversible crosslinks through covalent, non-covalent, or dynamic covalent bonding interactions. In this work, using equilibrium Langevin dynamics simulations we understand the relationship between the structure and viscoelasticity of a dually crosslinked RPN. We employ single-chain nanoparticles (SCNPs) to model the reversible polymers and dual crosslinking, where orthogonal crosslinkers (A and B) are introduced in the polymer backbone. SCNPs are attractive polymeric materials owing to their potential applications in drug delivery and catalysis, and comparable morphologies with intrinsically disordered proteins [2].

At infinite dilution, we find that the orthogonal cross-linking leads to more compact SCNPs, suggesting an effective approach for generating globular SCNPs.[3] In addition to the structure of the chains, we explored the role of weak (A-A) vs strong bonds (B-B) in tuning the stress relaxation behavior of the networks, by systematically varying the relative composition of A monomers (x), at a concentration where the system-spanning network will form.[4] Interestingly, we find a non-monotonic trend in the diffusivity and consequently in the stress auto-correlation function of the system w.r.t. x. In addition, we find that in the plateau regime, the dynamics is dictated by the strength of the weak bonds, whereas the terminal relaxation behavior of the stress auto-correlation function depends on the strength of the strong bonds. Further, we find that the distribution of the crosslinking monomers has a significant impact on tuning the stress relaxation behavior. We believe our results aid in understanding the interplay of weak vs strong bonds and the specific effects of their relative composition and distribution in tuning the viscoelasticity of the RPNs.

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PH-P9

Benzene tetracarboxylic acid doped polyaniline functionalized with graphene oxide: morphological and electrochemical characterization

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We report the preparation of benzene 1,2,4,5-tetracarboxylic acid (BTCA) doped PANI nanostructures functionalized with GO to investigate and enhance the supercapacitive behavior of the ternary nanocomposite BTCA/PANI/GO. BTCA plays the role of a dopant acid as well as a structure-directing agent. The system has been optimized and found BTCA: Aniline (An) to be 1:4 and An: APS (Ammonium persulphate) to be 1:1 (both are taken as molar ratio). The detailed morphological analysis suggests that GO has been functionalized uniformly among the spikes of BTCA/PANI. The SAED pattern confirms the presence of a polycrystalline structure of the ternary composite Almost 60% (weight) retention after 800 °C makes the composite thermally stable, and suitable for high-temperature applications. Electrochemical characterization indicates that the synthesized ternary composite BTCA/PANI/GO exhibits enhanced supercapacitive behavior, as evidenced by the increasing area under the cyclic voltammetry (CV) curve and increase in the maximum current with an increase in the scan rate. This behavior can be attributed to the capacitive properties of the composite. During the discharge cycle, the appearance of the ohmic drop is attributed to the contribution of double-layer capacitance. Furthermore, the conductivity of the ternary composite is found to be dependent on the molar ratio of BTCA to An, and follows the variable range hopping mechanism, providing valuable insights into the electrical transport phenomena in the composite material. BTCA/PANI/GO suggests improved π-π interchain stacking, which results in increased conjugation length, longer mean free path and finally supports improved carrier transport because of less structural disorder of the PANI chain.

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Self-assembly of A_2B Miktoarm Star Block Copolymer under Cylindrical and Spherical Confinements

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Block copolymers are exciting materials owing to their ability to self-organize resulting in ordered mesophases in bulk. A rich variety of interesting novel ordered phases can be obtained by subjecting the polymer to geometrical confinement. In the present study, we investigate the self-assembly behavior of A_2B star block copolymer melt under cylindrical and spherical nanopores using the self-consistent field theory (SCFT) [1]. In comparison to linear AB diblock copolymer, the branch architecture of A_2B block copolymer tends to influence the phase behavior. The structural frustration leads to various ordered phases such as single helix (H_1), double helices (H_2), triple helices (H_3), toroid with 3 spheres (TS_3) and concentric lamella (CL) in cylindrical nanopore. The role of introducing one additional arm of A block to a linear AB diblock copolymer in phase behavior is examined for different wall selectivity towards the majority component. First when majority B block likes the confinement surface and second for majority A block liking the confinement surface. When the branched component, that is A-block, is minority component and the surface prefers B-block, the region of helical phases transitions to the concentric lamella phase. However, for the case when the branched component is majority and prefers the confinement surface, the helical ordering of minority B-block is favored. The branched architecture of A_2B alters the phase behavior under spherical confinement vis-à-vis linear AB block copolymer.

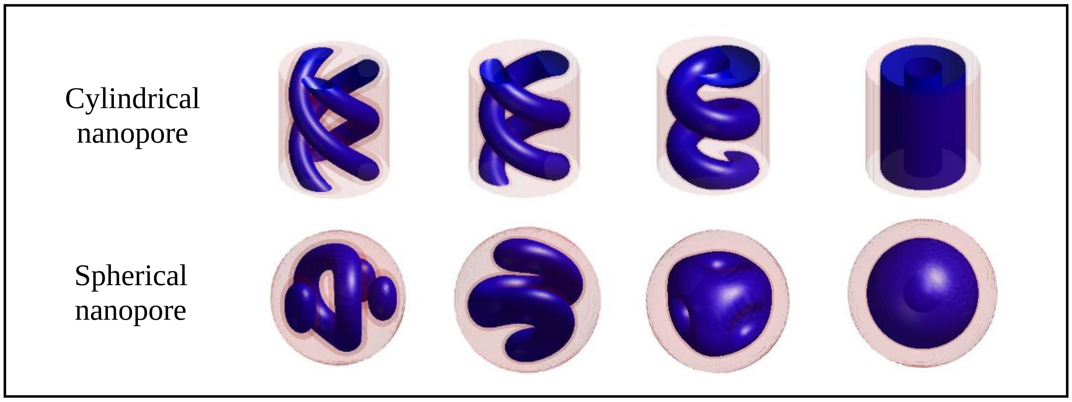

Figure 1: Typical ordered microstructures of A_2B miktoarm star block copolymer under cylindrical and spherical nanopores.

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PH-P13

Role of sequence on the phase behavior of thermoresponsive Copolymers

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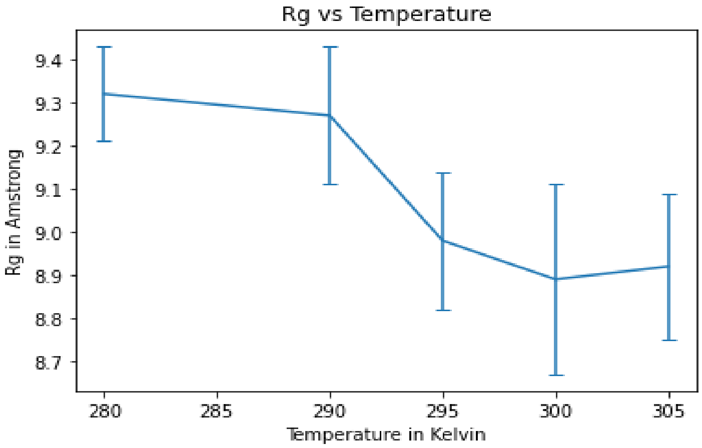
Thermoresponsive polymers such as poly(N-isopropylacrylamide) (PNIPAM) exhibit tunable properties and are promising materials for various technologies including biomedical applications, drug delivery and chromatography. The PNIPAM undergoes a phase transition in aqueous solution from a random-coil structural ensemble to a globule structural ensemble at the lower critical solution temperature (LCST). Engineering the LCST of PNIPAM is an active field of research. It is generally achieved by (i) variation of the chain length, (ii) introducing hydrophilic monomer units, e.g., N,N-dimethylacrylamide or other acrylamides to get a copolymer, (iii) altering the polymer tacticity, (iv) adding hydrated ions such as urea or cosolvents, and applying pressure. Among these, copolymerization produces an astronomically large number of sequences, and the impact of these sequences on the phase behavior is not well understood. Here, we conduct large-scale all-atom molecular dynamics (MD) simulations of NIPAM-based copolymers in water and establish correlation between its monomer sequence and coil-globule transition.



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Interaction of chitosan with water vapor: An experimental & simulation study

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Chitosan is a biopolymer-based hydrogel that can swell about a thousand times through the absorption of liquid water. However, upon exposure to water vapor, the swelling exhibited by chitosan is significantly diminished compared to its response to liquid water. Notably, free-standing chitosan films mounted in a cantilever configuration, exhibit a remarkable reversible actuation phenomenon upon encountering water vapor. A sequence of snapshots capturing a complete actuation cycle is presented in Figure 1(a). The physics behind this actuation behavior is commonly attributed to a differential swelling-driven mechanism. During water vapor exposure, a strain gradient develops across the thickness of the film, facilitating the observed actuation. We note that the durability and reproducibility of actuation performance are found to improve with crosslinking the polymer film and will be presented in detail.

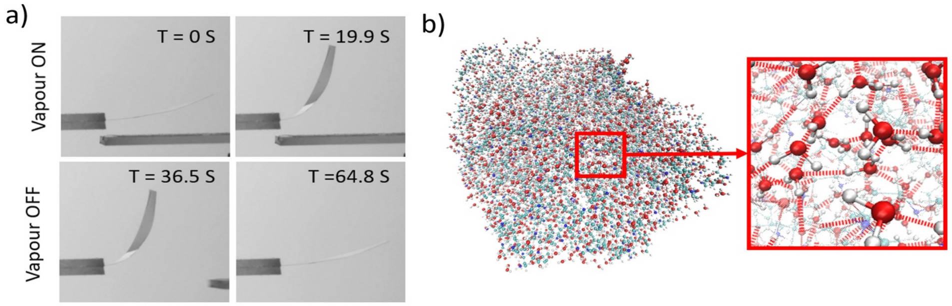

Figure 1: (a) Snapshots recorded during one actuation cycle of a chitosan film upon exposure to water vapor (crosslinking ratio: 0.012%, aspect ratio: 30μm x 15mm x 4mm). (b) Snapshot during simulation of bulk chitosan with 12k atoms interacting with water molecules.

To comprehend the reversible actuation mechanism arising from the interplay between chitosan molecules and water vapor, an all-atom molecular dynamics simulation study was undertaken. A snapshot of this simulation is depicted in Figure 1(b). The inset image shows the hydrogen bonds formed between water molecules (represented by red spheres for oxygen and white spheres for hydrogen) and chitosan, illustrated by dashed lines. Our main objective is to find out the distribution and dynamics of water molecules across the bulk and surface layers within the chitosan-water complexes. The simulation reveals a relatively higher accumulation of water molecules at the surface of chitosan molecules compared to bulk. These findings from the simulation also offer new insights into a *plausible actuation mechanism based on water vapor induced alterations in surface forces*. The detailed time evolution of water distribution provides information about the adsorption, permeation, and diffusion properties of water through the polymer matrix are also obtained. A quick rearrangement of the water molecules adsorbed to the surface on transferring to a dry atmosphere is observed in the simulation, which resonates with the experimental observation of relaxation of free-standing films to their original position upon withdrawal of water vapor.

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Effects of confinement on polymer translocation

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The study involves a comprehensive exploration of the intricate interplay between polymer translocation and confinement dynamics within a cone-shaped pore. A linear polymer chain is represented using the self-avoiding walk (SAW) model, effectively capturing the polymer's movement on a square lattice. The investigation involves manipulating the extent of confinement through two distinct ways: either by repositioning the back wall while maintaining a constant apex angle, or by adjusting the apex angle while keeping the back wall stationary. The notion of effective space φ, which quantifies the no. of monomers within the chain to the total available lattice sites within the cone. This φ value changes with different degrees of confinement, thereby directly impacting the dynamics of polymer translocation. The entropy of the confined system is analyzed as a function of φ, revealing non-monotonic behavior. Additionally, the free energy associated with confinement is calculated concerning a virtual coordinate. By utilizing the Fokker-Planck equation, the translocation time is computed , considering various solvent conditions across the pore. The findings indicate that the translocation time decreases as φ increases, eventually reaching a saturation point of φ. The study also suggests the potential for manipulating translocation dynamics by controlling the solvent quality across the pore.

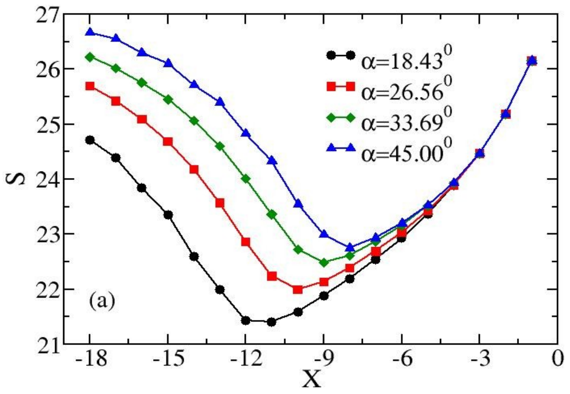

Figure: Variation of entropy S as a function of back wall position X for different apex angle

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Combined Electromechanically Driven Pulsating Flow of Non-Linear Viscoelastic Fluids In Narrow Confinements

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Controlled microscale transport is at the core of many scientific and technological advancements, including medical diagonistics, separation of biomolecules, etc., and often involves complex fluids. One of the challenges in this regard is to actuate flows at small scales in an energy efficient manner, given the strong viscous forces opposing fluid motion. We try to address this issue here by probing a combined time-periodic pressure and electrokinetically driven flow of a viscoelastic fluid obeying the simplified linear Phan-Thien-Tanner model, using numerical as well as asymptotic tools, in view of the fact that oscillatory fields are less energy intensive. We establish that the interplay between oscillatory electrical and mechanical forces can lead to complex temporal mass flow rate variations with short-term bursts and peaks in the flow rate. We further demonstrate that an oscillatory pressure gradient or an electric field, in tandem with another steady actuating force can indeed change the net throughput significantly - a paradigm that is not realized in Newtonian or other simpler polymeric liquids. Our results reveal that the extent of augmentation in the flow rate strongly depends on the frequency of the imposed actuating forces along with their waveforms. We also evaluate the streaming potential resulting from an oscillatory pressure driven flow and illustrate that akin to the volume throughput, the streaming potential also shows complex temporal variations, while its time average gets augmented in the presence of a time-periodic pressure gradient in a non-linear viscoelastic medium.

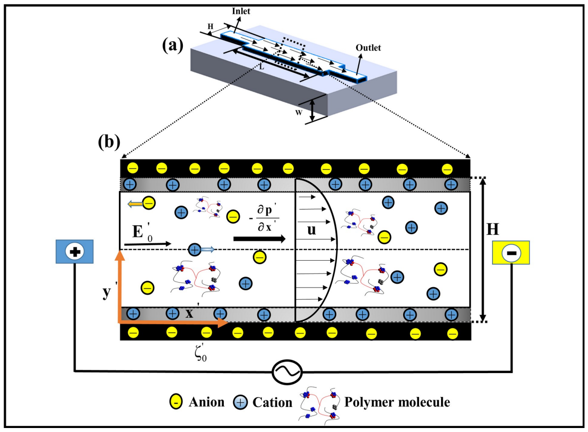

Figure 1: Schematic showing the physical systems under consideration. (a) Microfluidic deviece. (b) A channel of height H, which contains a viscoelastic fluid has been shown. The walls of the channel bear a surface charge and have potential ζ'_0. Flow is actuated using a combination of time-periodic pressure gradient and electric field.

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Role of Rheology on the Magnetic Field Orientation of Graphene Nanosheets in Polymers

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The isolation of graphene in 2004 by Novoselov and co-workers with the scotch tape method opened the doors to a new class of materials: 2D materials. Graphene gained interest rapidly due to its large-exposed surface area, high electrical and thermal conductivity, and excellent mechanical strength. Owing to these extraordinary properties, graphene has the potential to address some of the most critical global crises, including energy storage and a shortage of fresh water. However, one of the most critical challenges to be overcome, particularly in graphene systems, is the arbitrary functionality-driven orientation of the 2D nanofillers. While flow-induced structuring in graphene nanocomposites is widely applicable and relatively understood, flow fields are strong limiting factors for morphology. Therefore, in this context, we are exploring the orientation of graphene nanosheets in a polymer using an induced magnetic field. The behavior of the graphene nanosheets in a polymeric matrix under a magnetic field depends on its geometry, the strength of the magnetic field, the interaction of the graphene surface with the polymer solution/melt, and, essentially, on the rheological properties of the latter. While the role of rheology is sometimes underscored, the exact influence of rheological properties is not fully understood and is sometimes contradictory in the scientific literature. Therefore, here we focus on the orientation dynamics comparatively between the effects of time and shear rate in simple shear flow and the effects of magnetic field intensity and time for polymer solutions containing graphene nanosheets. To probe the orientation dynamics, we examine frozen (LN2) flow or magnetic field experiments to arrest the morphology at given experimental times. Furthermore, during simple shear we are also monitoring the electrical conductivity of the solutions via simultaneous steady shear and dielectric spectroscopy, whereby the DC conductivity can be determined in the limit of low electrical frequencies.
We consider the effect of graphene concentration and polymer solution composition and determine their effect on the shear rheology, viscoelastic properties and yield stress of the samples and, subsequently, their orientation dynamics.

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PH-P18

Comparisons between Free Monomer Clusters and Polymer Globules by using molecular simulations.

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Studies on the conformations of polymers are very important for predicting the natural properties of the polymers in solutions and also help in designing polymers that respond to stimuli.[1] For example, it could help in designing polymeric adsorbents that respond to the presence of small molecules. Previous studies have considered polymer conformational change as a phase transition and compared it to fluid-fluid transition.[2][3] This presentation intends to show the efforts to compare polymer conformational change to liquid-liquid phase transition with the help of molecular simulations. Molecular Dynamics simulations of bead-spring model of polymer were carried out in an explicit solvent. Both monomers and solvents are taken to be Lennard Jones particles. To study liquid-liquid phase transition the simulations of free monomers are carried out in semi-grand canonical simulation by Monte Carlo method. Clusters formed in free monomer simulations are then compared to polymer globules that are formed in polymer simulations. The noticeable result is that for poor solvents the Polymer globules and Free Monomer Clusters, radii of gyration are quite similar. The same was the case for Radial Distribution Functions between Monomer-Solvent molecules. This indicates there is a similarity between liquid-liquid phase transition and polymer collapse for poor solvents. Further research shows that bonded interactions in the polymers in liquid solutions have a similar effect as impurities in heterogeneous nucleation during liquid-liquid phase transition.

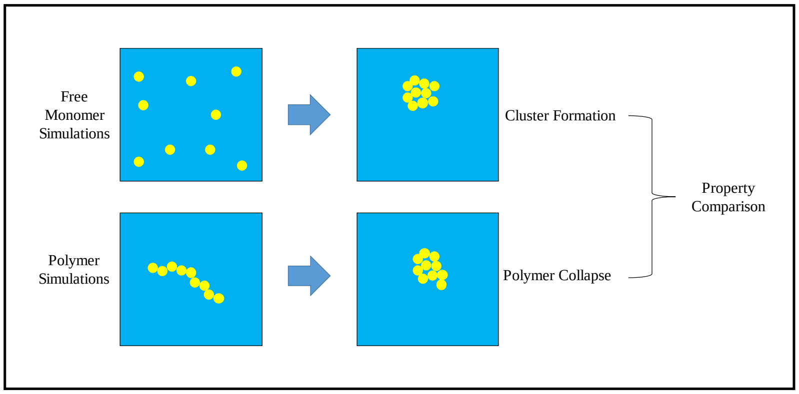

Figure 1: Visual Representation of polymer and free monomer simulations with cluster formation and polymer collapse

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Influence of Ca^{2+} Ions on Rheological and Dielectric Behavior of Sodium Carboxymethyl Cellulose (NaCMC) and Esterified Hydrogels

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Polyelectrolyte-based conductive hydrogels are being extensively explored for applications in biomedical, tissue engineering, water purification and the fabrication of multifunctional soft materials. We synthesized ionically crosslinked, esterified, and Ca^{2+} doped esterified hydrogels based on sodium carboxymethyl cellulose (NaCMC), and the influence of Ca^{2+} ions have been studied to understand the structure-property relationship. It is found that Ca^{2+} ions have an important role in determining the rheological and dielectric response of hydrogels. Storage modulus for ionically crosslinked and esterified NaCMC was enhanced. However, a decrease in storage modulus was observed for Ca^{2+} doped esterified hydrogels with the addition of Ca^{2+} ions. Power law behavior was observed in their rheological responses. NaCMC based ionically crosslinked hydrogels have relaxation times in the range of 8.9×10^{-5}s - 2.8×10^{-5}s may be due to the formation of temporary dipoles by electrostatic bridge formations, whereas, esterified hydrogels showed relaxation times in the range of 10^{-3} s - 8.9×10^{-5} s with increasing ester crosslinks. Interestingly, Ca^{2+} doped esterified hydrogels showed multiple dielectric relaxations on Ca^{2+} ion addition with different relaxation times may be due to change in ionic environment around polyion chains.

Keywords: Hydrogels, Broadband Dielectric Spectroscopy (BDS), Rheology

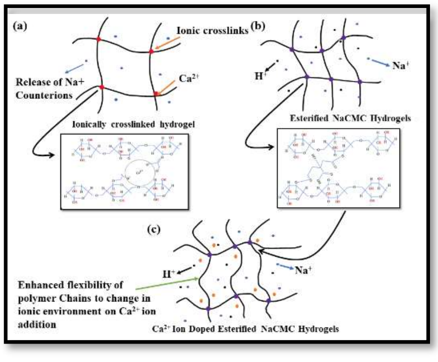

Figure 1: Schematic Representation of Ca^{2+} Ion Doped Ionic and Esterified Hydrogels

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PH-P20

Salt-dependent swelling kinetics of polyelectrolyte gels

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Polyelectrolyte gel is a subclass of polymer gels where the polymer backbone contains ionic groups. In presence of the solvent in the gel, these groups dissociate to release small ions (counterions) into the solvent. Polyelectrolyte gels are characterized by their large swelling ratios due to counterion pressure and electrostatic repulsion between charged backbone segments. In the present work, we have theoretically modeled the swelling kinetics of polyelectrolyte gels for different environmental salt concentrations. This is useful for predicting their swelling behavior in physiological environments which often contain salt. We numerically solve the force balance equation [1] for the gel, derived from theory of elasticity, by rewriting the Osmotic stress [2] using free-energy expression [3]. The free energy is a function of free ion concentration in the gel, which is derived as a function of environmental salt concentration(c) using the theory of Donnan equilibrium [4]. In agreement with experimental observations [5], for higher salt concentrations - the equilibrium swelling degree is lower and the gel reaches equilibrium faster. The spatial and temporal variations of polymer concentration, degree of ionization, osmotic pressure and free ion concentration within the gel are obtained for different values of c. For small proportional changes of c, the comparison of the kinetics reveals a particular scaling behavior which enables us to model the swelling curves using simple mathematical expressions.

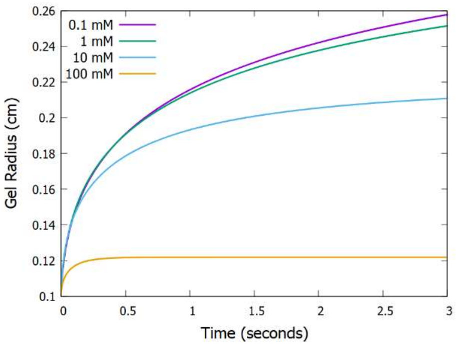

Figure 1: Swelling behavior of polyelectrolyte gel for different salt concentrations.

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PH-P21

Pattern formation in electro-responsive polymer ionic liquid blends

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Self-assembled patterns obtained by controlling the reaction-diffusion (RD) phenomena through external stimuli, have been extremely useful for designing multifunctional synthetic soft materials. Here we develop a mechanism that harnesses contactless technique to self-assemble intricate patterned domains in incompatible polymer ionic liquid (PIL) blends via uniform electric field. Through modelling and simulation, we demonstrate that RD can be directed by electric field that ultimately, results in the formation of phase separated PIL domains in an organized manner. Our RD model is based on Poisson Boltzmann Nernst Planck (PBNP) equations that incorporates long-range electrostatic interactions between charged moieties through Boltzmann distribution in both, the strong and weak segregation limits. In addition, we quantify the domain growth, characteristic domain size and phase ordering by calculating circularly averaged structure factor (S) as depicted in the figure below.

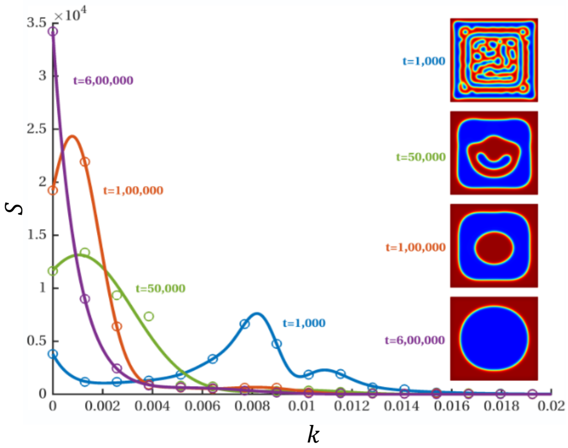

Figure: Time evolution of the morphology of the PIL system with electric field applied at all the boundaries and the corresponding circularly-averaged structure factors ($S\ vs.\ k$).

The figure illustrates that, with the advent of time, the structures enlarge from thin lamellar morphology into two well-segregated large domains, comprising polymer-rich and ionic liquid-rich phases. We also establish that the striped patterns of different thicknesses are formed depending upon the segregation of PIL-domains. In essence, the resolution of the formed patterns is primarily governed by the segregation between the PIL domains. Ultimately, we demonstrate that different ordered arrangements of PIL domains can be obtained from one setup by changing the direction of the electric field and quenching the system. On the whole, our method, despite being non-contact, is quite versatile and robust and can be utilized to create networked microstructures that can be used for micro-scale fabrications, including the manufacture of electrochemical, energy-efficient and microfluidic devices, actuators, etc.

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PH-P22

Dynamics of interior loop formation in polymer chains: effect of tail length and confinement

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The process of two distant segments of a polymer chain making a loop is an elementary process for many biological functions. While the majority of previous studies have considered end-loop formation, interior-loop formation is more common in vivo. We investigate the loop formations between two inter-segments of length l with dangling tails of length l_t for both ends (so the total chain length $L = l + 2l_t$). For a given inter-loop length l, the looping time increase sharply as $T \sim l_t^{\alpha}$, with $\alpha \simeq 1.5$. This finding indicates that for a very long tail, the loop formation time would be prohibitively long. However, in the presence of external confinement, T (l_t) is saturating above a certain value of l_t. To rationalize this behavior, we analyze the diffusive behavior of the chain monomer in the presence of confinement.

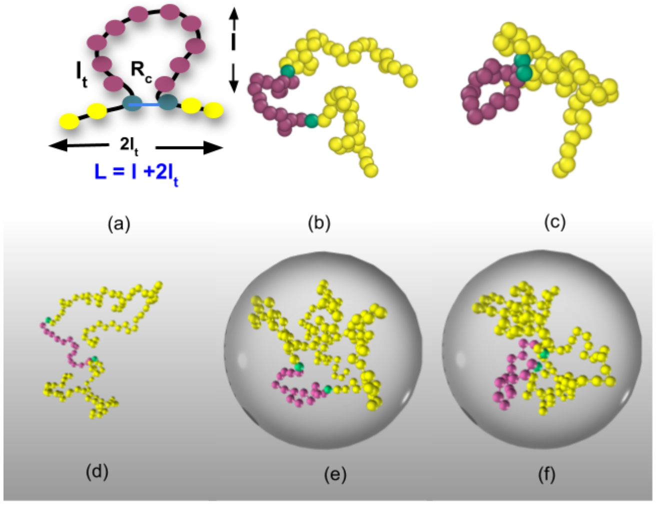

Figure 1: Internal loop formation. (a) Schematic illustration of a model of polymer loop formation. (b), (c) and (d) Model of polymer interior loop formation in a free environment. (e) and (f) Internal loop formation of a polymer chain inside spherical confinement.

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Thermal melting and force induced unzipping of DNA hairpin: Unfolding pathways and phase diagrams

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We have studied the thermal melting and force induced unzipping of a DNA hairpin on the face centered cubic lattice by using the exact enumeration technique for two different sequences which differ in terms of loop closing base pairs. The melting profiles obtained from the exact enumeration technique is consistent with the Gaussian network model and Langevin dynamics simulations. Probability distribution analysis based on the exact density of states revealed the microscopic details of the opening of the hairpin. We showed the existence of intermediate states near the melting temperature. The force extension curves show mechanical properties (stability) of the sequence, which differ from the thermal melting. We further showed that different ensembles used to model single molecule force spectroscopy setups may give different force-temperature diagrams. We delineate the possible reasons for the observed discrepancies.

Figure 1: Schematic representations of a ssDNA hairpin on a face-centered cubic lattice system. (a) represents the native structure of a stem-loop hairpin structure; (b) shows the formation of bubble during the melting of hairpin. (c) corresponds to the open state of the hairpin.

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Predicting Phase Behavior of Polymer-Nanorod Composites Via Coarse-Grained Molecular Dynamics Simulations

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Polymer nanocomposites are very well-known for their tunable mechanical, electrical, rheological, and many other properties. These tunabilities are attributed to the nanoparticle distribution within the polymer matrix. For example, recent experiments suggest that electrical conductivity of a polymer matrix can be tuned to a large extent with the addition of nanorods in it. However, the mathematical correlation between the nanorod distribution in a polymer matrix and its electrical conductivity reinforcement is not fully understood. To establish the underpinning molecular mechanics, we perform large-scale coarse-grained molecular dynamics (MD) simulations of a phenomenological model nanorod-polymer system. We model the polymers as fully flexible bead-spring chains within the Kremer-Grest framework, and the nanorods are represented as rigid bodies that are made of the Lennard-Jones beads [1]. All simulations are conducted in isothermal-isobaric ensemble within the LAMMPS MD environment [2]. Our simulations suggest the formation of a percolating network-like distribution of nanorods with the increment of their concentration. We infer that this percolation leads to the enhancement of electrical conductivity. In addition, we study the change in nanorod distribution when polymers are crosslinked. We also establish a phase diagram of the composite as a function of nanorod concentration and nanorod-polymer size ratio. This phase diagram suggests nanoparticle dispersion, percolation, and complete phase separation depending on nanorod concentration and nanorod-polymer size ratio. The MD snapshots for two representative phases are shown in Figure 1. Overall, our work provides a molecular mechanism of the tunable electrical conductivity of a polymer matrix.

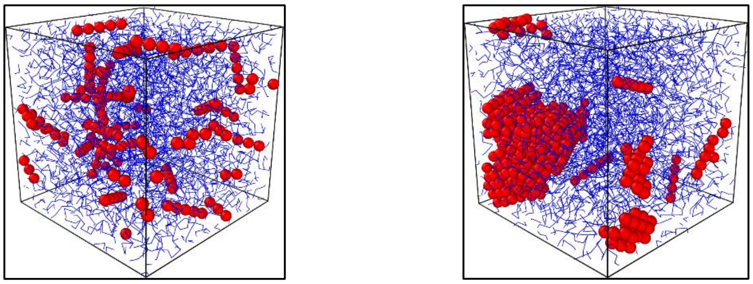

Figure 1: MD snapshots demonstrating nanorod (a) dispersion and (b) microphase separation for nanorod concentration 0.02 and 0.07, respectively. The red beads correspond to nanorods, and blue chains correspond to polymers.

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Investigation of cone shape parameters in polymer electrospinning via *in situ* visualization: towards precise control over fiber diameter

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Electrospinning is a polymer processing technique in which a high voltage is applied to a polymer solution flowing through a metal orifice. As the voltage is increased, the spherical polymeric droplet transforms into a cone, and a jet emerges from its apex. The jet undergoes bending instabilities before depositing on a grounded metal collector as a non-woven mesh. Controlling fiber diameter is of critical interest in electrospinning due to its importance in the successful use of electrospun meshes. Towards the long-term goal of achieving direct control over fiber properties, our strategy is to study real-time changes to the charged cone and jet because specific cone/jet features have previously been shown to correlate with fiber properties. In this study, we visualize poly(caprolactone) (PCL) electrospun from two different solvents under different system/operating conditions, such as solution concentration and voltage. We identify unique cone shapes in the stable cone-jet mode through *in situ* visualization and characterize them with respect to changes in the curvature (k), Taylor cone height (L_c), and initial jet diameter(d_{ji}). The shapes are analyzed using a custom MATLAB code developed in-house with the boundary is extracted from the raw images. We also reveal correlations of specific cone-jet features with fiber diameter. By leveraging these shape analyses, fiber diameter on the collector can potentially be modulated and tightly controlled as required in diverse applications.

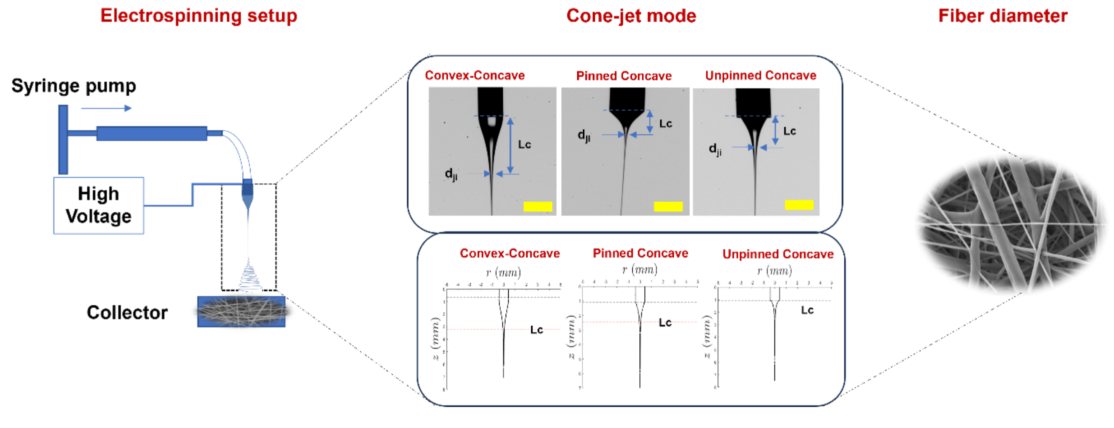

Figure 1: Strategy used for studying cone shapes in polymer electrospinning

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Indian Society of Rheology

Improving functional Properties of PNIPAM hydrogel using extracted seed mucilage of Salvia Hispanica

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Smart hydrogels made of crosslinked poly(N-isopropylacrylamide) (PNIPAM) chains are widely investigated owing to their reversible volume phase transition close to human body temperature[1]. Native pNIPAM hydrogels possess application prospects in the field of targeted and controlled drug delivery[1]. Here, we investigate methods to augment the swelling behavior and mechanical properties and biocompatibility of PNIPAM-based hydrogels by incorporating naturally derived biopolymers sourced from *S. Hispanica*, a widely employed gelation agent and vegan thickener in food products[2]. We observe that the interpenetrating polymer network of PNIPAM and *S. Hispanica* mucilage yields composite hydrogels that manifest improved water absorption, swifter swelling kinetics, and elevated swelling ratios in comparison to pure PNIPAM hydrogel[1]. Effect of crosslinking density and the amount of *S. Hispanica* mucilage in the composite hydrogel on its swelling kinetics is also presented. Further, we also investigate the rheological properties of the native and composite hydrogels to understand the viscoelastic properties of the hydrogels and deduce information about the nature of cross-linking present within the hydrogels. Efforts are also underway to enhance the volume phase transition temperature of the composite hydrogel from that of native pNIPAM hydrogels in order to bring it closer to human body temperature.

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Novel Evaporation Kinetics of a Droplet Containing Polymer

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A comprehensive understanding of the kinetics of sessile drop evaporation provides valuable insight into numerous phenomena and finds application across various domains such as coating and printing, diagnostics and sensing, self-assembly, microfluidics, and biomedical application. Typically, a fluid droplet, roughly the size of the capillary length, evaporates through a constant contact radius (CCR) mode, a contact angle (CCA) mode, or a combination of both. Here, we report a novel observation of the evaporation kinetics of a polymer-loaded droplet placed on a high-energy hard solid surface. Intriguingly, as the droplet undergoes evaporation, its contact angle increases. Notably, this peculiar phenomenon is observed in droplets with initial contact angles within a specific range, approximately 20 degrees. Interestingly, the increase in contact angle also accompanies a continuous slippage of the three-phase contact line of the droplet during the evaporation process. To validate this contact angle increase, we employ two independent measurement techniques: Shadowgraphy for optical visualization of the droplet and the refraction of light from the Fringe projection method. The observed increase of the contact angle during evaporation is corroborated by considering the volume change induced by slippage and the rate of solvent molecule evaporation. The effect of polymer concentration and its molecular weight, and on the evaporation kinetics and generality of this observation will be presented in detail.

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Tuning Thermal conductivity in bottlebrushes: A molecular dynamics simulation approach

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Using large scale molecular dynamics simulation of a generic model, we investigate heat flow in bottlebrush polymer systems. In bottlebrush polymers, a linear chain (backbone) is grafted with side chains at grafting density, ρ_g. Both the side chain-length, N_s and ρ_g strongly influence the backbone chain stiffness. Thermal transport coefficient, κ in a branched polymer strongly correlates with backbone stiffness. We present the effect of N_s and ρ_g on κ for bottle-brush polymers. The results from our molecular dynamics simulation show that κ has a non-monotonic dependence on ρ_g. We also find that longer side chains lead to reduction in κ, indicating that molecular vibrations and phonon scattering have a significance role. These results not only help us to learn more about how heat current flow through complex polymer system, but also give us substantial insight into how to design bottlebrushes with desired κ for various applications.

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Polyethylene grafted sheet-like silsesquioxane nanocomposites with unprecedented adhesion to polar substrates

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Polyethylene (PE) is one of the most widely used commodity polymers. However, its apolar nature limits its functionality, particularly its adhesion properties necessitating tie layers in multilayer product architectures. Thus, there is a growing interest in developing functional polyethylenes that adhere to various substrates without needing tie layers. In this study, we report a clay-like layered Mg-silsesquioxane (NB-sil) grafted with polyethylene chains from its surface (PE-sil). XRD indicates that NB-sil has a sheet-like structure analogous to a 2:1 phyllosilicate with an octahedral brucite-like sheet sandwiched by two tetrahedral silicate sheets. These silsesquioxanes are defected, and resemble a crumpled sheet with a lateral size of ~ 0.5 μm.

This novel nanocomposite, with less than 2 % by weight of the inorganic content, exhibits unprecedented adhesion towards polar substrates like metal and glass. We measure bonding strength of ~ 100 MPa to stainless steel and aluminum, 100-fold higher than for polyethylene (Figure 1a).[1] Enhanced adhesion is attributed to the higher polarity of the samples. Although the polyethylene nanocomposite exhibits increased polarity, the polyethylene nanocomposite is compatible with a polyethylene matrix and exhibits co-crystallization (Figure 1b).

These properties suggest potential applications of the polyethylene nanocomposite as hydrophobic adhesives and sealants, etc.

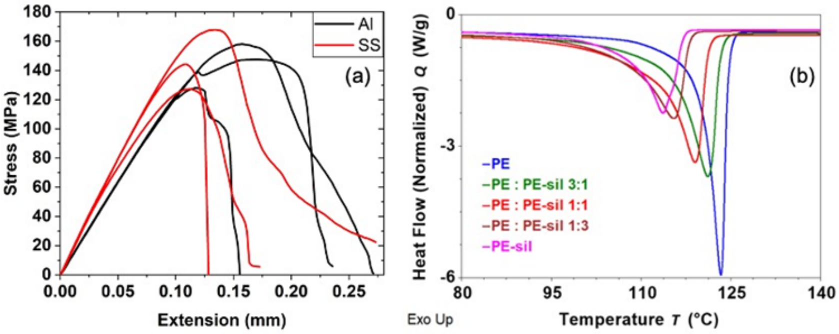

Figure 1: (a) Bonding strength of PE-sil against aluminum (Al) and steel (SS). (b) Non-isothermal melting transitions of PE and PE-sil blends.

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Rheological studies on seed mucilage layers

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The polysaccharide complex exuded by seeds referred to as seed mucilage is used in many food-based applications. The seed mucilage also has many functions in nature such as in germination and seedling growth. The major constituents of seed mucilage include polysaccharides, such as, pectin, cellulose, hemicellulose and starch occasionally. Seed mucilage of certain species such as *Arabidopsis thaliana* and *Plantago ovata* have been reported in literature to have layered arrangement of mucilage, with each layer differing in composition and properties [1], [2]. In the current study, we explored such layered arrangement in sweet basil (*Ocimum basilicum*) seed mucilage by collecting the fresh mucilage obtained from hydrated seeds. Oscillatory shear and steady shear rheological studies are carried out on the weakly adhered mucilage layer (WA-BSM) and the strongly adherent mucilage layer (SA-BSM) to understand the differences in layered arrangement in basil seed mucilage. We explore the structural differences contributing to the rheological response of these layers and its biological significance.

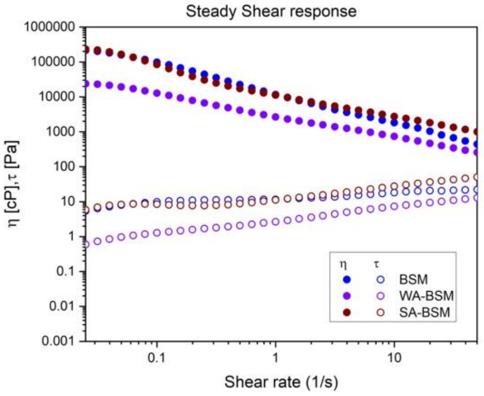

Figure 1: Steady shear response of WA-BSM, SA-BSM and BSM

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Soft and adhesive alginate hydrogel: Microstructure from MD simulations

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Alginic acid-based hydrogels have attracted much attention over the years for their therapeutic and mechanical applications. Our recent work has shown that Alginate ($[\text{Alg}]^-$) polymer chains crosslinked with a biocompatible organic cation (BOC) can form a soft, free-standing film having tunable bending ability, surface adherence to various tissues, and significant antibacterial activities. In-situ synthesis of silver nanoparticles using [BOC][Alg] has revealed its application as an anti-bacterial surface coating agent. It was found that the size and shape of the synthesized nanoparticles have an interesting dependence on the dilution of [BOC][Alg] polymer melt.

In this work, we perform all-atomic molecular dynamics (MD) simulations of [BOC][Alg] using the OPLS/AMBER force field. We used the LAMMPS program to successfully reproduce several physical properties (e.g. density, Tg) of pure Alginic acid to validate our model. At different concentrations of water, we investigate the changes in physical, mechanical, and rheological properties of [BOC][Alg] and compare them with $[\text{Na}^+][\text{Alg}]$ and $[\text{Ca}^{2+}][\text{Alg}]$. To understand the effect of water at the microscopic level, we analyze the micro-networks formed by the water molecules inside the polymer matrix. We further investigate the aggregation properties and hydrogen bond networks of [BOC][Alg] in an aqueous solution, which can be correlated to different nanoparticle sizes found in the experiment. Our work highlights the unique influence of BOC crosslinkers on the microstructural and mechanical properties of the alginate hydrogel.

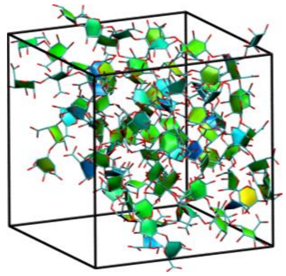

Figure 1: Pure Alginic Acid (10-mer) with M/G=1.5

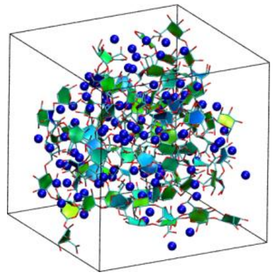

Figure 2: $[\text{Na}^+][\text{Alg}]$ (10-mer) with M/G=1.5

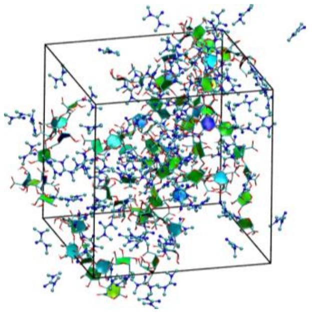

Figure 3: [BOC][Alg] (10-mer) with M/G=1.5

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Low pH self-organisation of similarly charged Polyethylenimine chains into light-responsive microstructures.

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Polyethyleneimine (PEI), an amine containing weak polyelectrolyte has emerged as a fascinating candidate for designing advanced materials with tailored properties and functionalities due to the presence of versatile interactions in it. It has the tendency to form polyplexes by electrostatically binding with oppositely charged small molecules or macromolecules, such as nucleic acids (DNA and RNA). These polyplexes find applications in gene transfection or drug delivery. The main driving force behind PEI's potential lies in its highly charged nature, resulting from the presence of primary, secondary, and tertiary amines. However, all amines do not become fully protonated even when the pH of the PEI solution is lowered to 1. This distinctive behavior leads to PEI's remarkable buffering capacity, referred to as the "proton sponge" effect, that makes it the gold standard candidate for non-viral gene transfection. Our research has unveiled truly unprecedented assembly of 70% protonated PEI chains into hollow, robust fibrillar network at pH around 3. Further, by sparsely incorporating dyes such as Fluorescein Isothiocyanate(FITC) or Rhodamine Isothiocyanate(RITC) into branched PEI chains, we have demonstrated their spontaneous assembly into fibrillar and sheet-like structures. This phenomenon can be primarily attributed to a combination of proton-sponge effect of PEI chains and excited state proton loss from the covalently attached fluorophores. Through the use of specific wavelengths of light, dye-polymer interactions are initiated, leading to the creation of structures resembling bead necklaces in fibers or the collapsing of sheets.

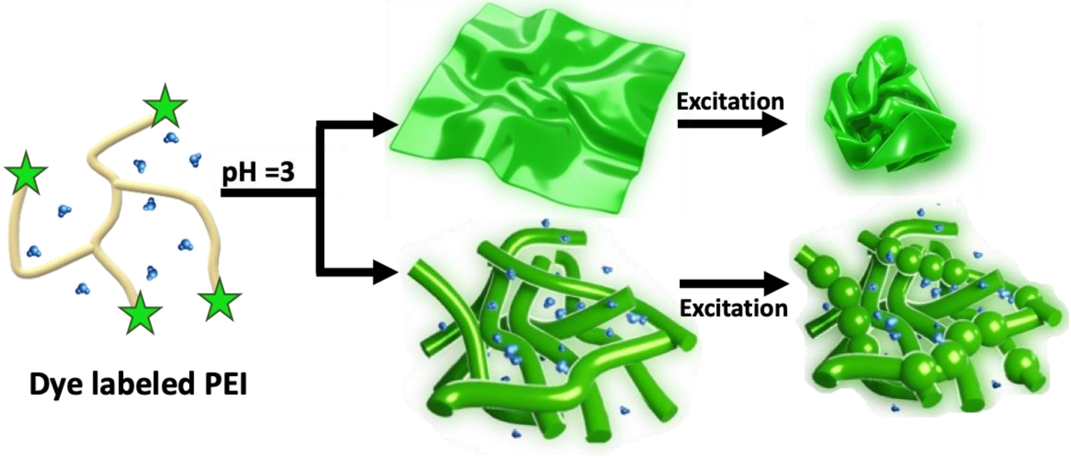

Figure 1: Light responsive behaviour of PEI-dye assemblies at pH=3.

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Spreading and Evaporation of a Polymeric Droplet Impacting on Nonporous Substrate

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Transdermal drug delivery has emerged as a promising alternative to traditional routes of drug administration, offering advantages such as sustained release, improved patient compliance, and reduced systemic side effects. In this context film-forming sprays (FFS) have gained significant attention due to their advantages over other routes such as patch, gel, etc. In spray application, the drug is administered via an excipient such as ethanol, while polymers are added as drug release rate controlling agent and to prevent crystallization. The impact of the spray droplets on the skin leads to formation of a film, and the film thickness, uniformity, and evaporation rate of the solvent directly influence the transdermal drug penetration rate. Thus, understanding on the spreading and evaporation phenomena following impact of a single polymeric droplets is important for performance improvement of the FFS. However, most studies are based on sessile droplets. The primary objective of this study is to investigate the effect of addition of a polymer in ethanol on the spreading and evaporation behavior of the droplet upon its impact on a nonporous glass substrate. Eudragit E100 was selected as the polymer because of its good skin tolerance in clinical trials, and a 10% w/v polymeric solution of ethanol was prepared. Figure 1 shows the schematic diagram of the experimental setup. Experiments are conducted for both cases, viz. droplet impacting the substrate with a finite velocity and the sessile droplet. For the impact case the height of the free falling is controlled such that splashing is avoided in all cases. Utilizing a camera, top-view images of the drop impact are captured and subsequently processed in Matlab to calculate the droplet diameter and spreading/evaporation rate. In the experiments based on the impact of pure ethanol droplets (see Fig 2 which shows a time sequence of images), four distinct regimes are identified in the plot for time evolution of droplet diameter, namely, inertial, spreading, slow contraction, and rapid contraction, as shown in Figure 3. Interestingly, it is observed that the spreading rate and evaporation time are smaller for the impact cases compared to the sessile droplet. Currently research is underway to examine the influence of the polymer on different impact regimes following the impact of the plyometric droplet.

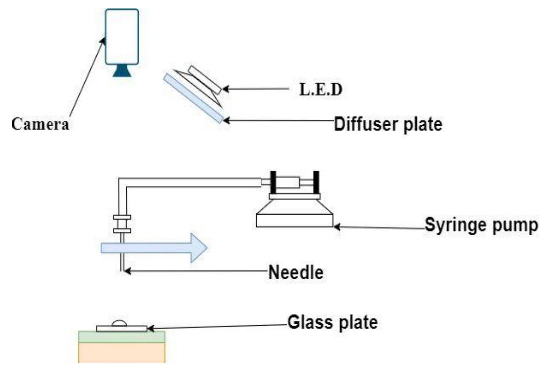

Figure 1: Diagram of the experimental setup

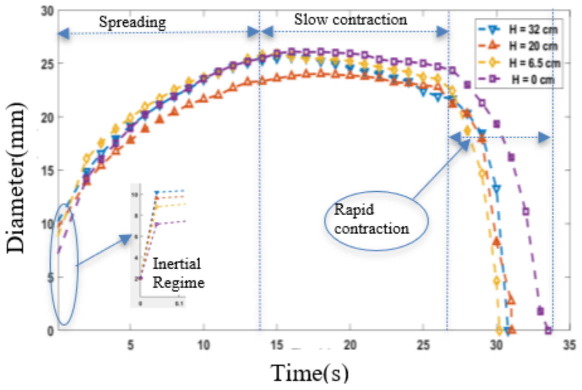

Figure 2: Time variation of droplet diameter with time

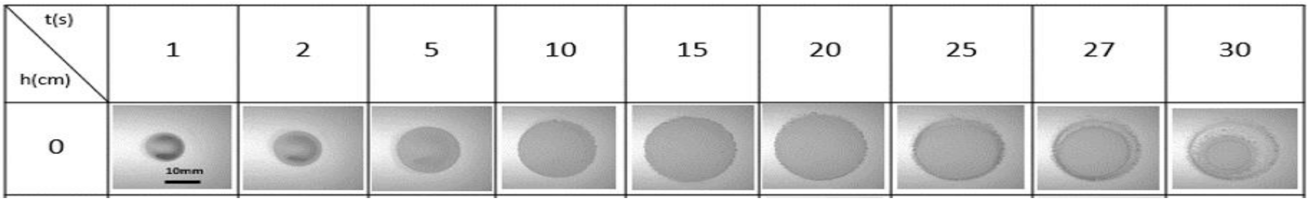

Figure 3: Time sequence of images of droplet after impact

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Particle image velocimetry as a tool to investigate lubricating effect of root mucilage

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To penetrate soil, a growing root must displace adjoining soil particles to make way for the increasing root volume. One of the key players in this natural phenomenon is a biopolymer in the form of a soft gel called mucilage, exuded primarily by the root cap. Mucilage reduces friction at the root-soil interface, thereby reducing root penetration resistance. A mechanical equivalent of this is penetration into soil by a penetrometer. The ensuing soil deformation patterns give insights about the mechanical efficiency of penetration. Soil deformation in the radial direction akin to an expanding cylinder has been found to be less energy intensive than deformation in the axial direction akin to an expanding sphere. Particle image velocimetry, which has its genesis in experimental fluid mechanics is a non-intrusive displacement measurement technique and has been employed in this study to visualize as well as quantify velocities of soil particles in the vicinity of growing roots. Decapped roots triggered responses in the rhizosphere aligning closer to the expanding sphere model and thus faced greater mechanical resistance. Conversely roots with their caps intact displaced soil particles similar to the expanding cylinder model, soil particles moved more easily around them reducing frictional resistance.

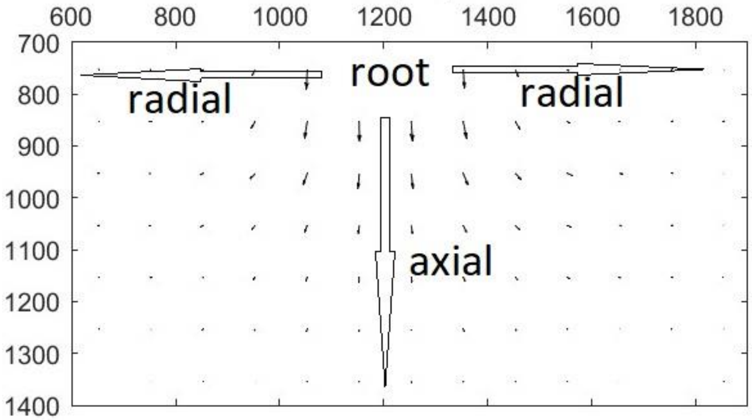

Figure 1: Soil displacement for green gram root with its cap removed. Co-ordinate units are pixels.

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Predicting Mechanical Properties of Biodegradable Copolymers using Molecular Dynamics Simulations

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Biodegradable and biocompatible elastomers have gained widespread attention in regenerative tissue engineering and drug delivery applications. Artificial 3D scaffolds of these polymers are expected to have tunable elastic properties, suitable biodegradation rates, and enhanced cell adhesion and proliferation. In this regard, Citric acid and diol-based copolymers are promising candidates as they combine high mechanical properties of synthetic materials and high degradability of biomaterials. The condensation polymerization between the inexpensive and water-soluble citric acid and 1,6-hexanediol leads to the formation of Polyester ethers (PEE). However, the correlations between PEE's mechanical properties, degradability, and molecular composition are poorly understood. Here we perform all-atom equilibrium molecular dynamics (EMD) and non-equilibrium molecular dynamics (NEMD) of Citric acid-1,6-Hexanediol copolymers and establish correlations between their structure and degradation for varying acid-to-alcohol ratio and the monomer sequence. The OPLS interatomic force field is used to model the copolymers. The data suggest a strong correlation between the elastic properties and the composition of the copolymers. The work provides essential design rules of PEE for artificial scaffolding applications.

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Novel composite hydrogels with enhanced thermal stability and injectability

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Interactions between the colloidal particles and the amphiphilic species play a major role in determining the overall microstructure of the composite systems. The effect of the addition of hematite pseudocubes/ akaganeite (β-FeOOH) nanorods in PF127 triblock copolymer solutions on the viscoelastic behavior, elastic strength, mechanical fragility, thermal stability, enhanced injectability etc., of the composite gel is studied through linear and nonlinear rheological behavior of this composite system. Even at small concentrations, the presence of β-FeOOH NRs can modify the strength and flexibility of PF127 gels. External magnetic field is used to tune and control the chain-like microstructures of hematite cubes in the composite gels. These gels show thermoresponsiveness and enhanced injectability, and could find applications in tissue engineering and drug delivery.

Figure 1: Composite hydrogels containing small amounts of paramagnetic akaganeite (β-FeOOH) nanorods in PF127 triblock copolymer show enhanced thermal stability and injectability which could find applications in tissue engineering and drug delivery.

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Adsorption of pH responsive ampholytic ions into a weak PE brush: A simulation study

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In the recent past polymer brushes , constituting a densely packed sequence of polymers with one end tethered to a surface has been investigated a lot due to their interesting applications in both industrial and biomedical research . One specific functionality is the use of charged polyelectrolytic brushes in the adsorption of globular proteins[1]. The strong electrostatic interaction from the densely packed brush results in substantial uptake of these modular proteins, even beyond the isoelectric point where both the brush and the protein are similarly charged. Works done on BSA protein adsorption into spherical[1] or planar brushes[2] attribute this to the lower effective pH in the interiors of the brush compared to the bulk which instigates a charge reversal of the ampholytic protein whenever it comes in the interactive influence of the chain[1,4] . They further speculate the role of oppositely charged patches on the protein surface which adheres to the brush interior concomitant with a huge favorable counterion release.

We study a two phase weak PE brush system in contact with an ionic reservoir consisting ionizable and pH-responsive ampholytic entities. The PE brush is simulated using a coarse grained molecular dynamic simulations and the acid-base equilibria of the brush as well as the exchange of ions across the two phases are implemented using the Grand Reaction Monte Carlo method[3]. The charge regulation inside the brush is dictated by the electrostatic contributions from the chain and the donan partitioning of ions across the two phases due to the electroneutrality condition . Here , the later especially in case of a densely packed system like PE brushes might substantially shift the effective pH inside the brush, which in turn might profoundly couple with the ionization state of the ampholytic ions and their overall uptake into the brush. Also, insights gained from the adsorption mechanism of these small ampholytic ions under changing physilogical conditions like pH, salt concentration , ampholytic ion concentration ,valency can be extended to more realistic cases of globular proteins like BSA where along with the charge regulation the structural arrangement of the ionizable side groups might bring interesting facets .

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Effect of Degree of Confinement on Mechanical Properties of Polymers Through Free Volume.

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The geometrical confinement of polymers, their impact on mechanical properties, and free volume characteristics have emerged as a crucial area of research in the field of polymer science. The mechanical and thermal behaviour of confined films drastically differs from their bulk counterparts. In the present study, we investigate the interplay between the degree of confinement in the polymer matrix and its effect on mechanical properties by analysing the free volume characteristics. In addition, quantitative comparison of free volume in bulk and the confined polymer systems were done. MD simulations to help understand mechanical properties by studying the relaxation characteristics and the free volume effect (morphology and distributions). The findings of this study expand our understanding of the fundamental concepts guiding polymer behaviour under different degrees of confinement and open new avenues for material design with applications ranging from sophisticated nanocomposites to biomedical devices.

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Solvent-assisted ink-based 3D printing of free-form structures via phase separation

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Soft material-based 3D-freeform structures are inevitable in soft robotics, a growing field of technology. Conventional 3D printing of thermoplastics by high-temperature extrusion methods is well established. However, fabrication of free-form 3D structures from solution-based precursors is still challenging. Here, we design structures based on non-solvent-induced phase separation in a tertiary system via direct ink writing. The thermoplastic polyurethane/dimethyl formamide (TPU/DMF) system is utilized as model ink for 3D printing in an aqueous medium. The main highlight of this work lies in the unique approach that incurs the 3D printing of soft polymers in the solution phase in a liquid bath that is not only miscible with the solvent ink component but also incompatible with the polymer. This leads to the spontaneous solidification and formation of strong vertical and horizontal interlayers without any extra support structures. This method offers a simple route to fabricate 3D free-form structures of a soft polymer, which can serve as a useful technique for DIW-based fabrication of soft robotic components and flexible wearable devices, as well as in-vivo organ and scaffold printing.

Keywords: direct ink writing, free-form structures, phase separation, thermoplastic polyurethane, soft biopolymer

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RS-O4

pH Responsive Actuators: Controlling Actuation Direction & Printing

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Stimuli responsive polymers and hydrogels are finding diverse applications in different fields, of special mention are wearable electronics and biomedical engineering. It’s extremely low weight to volume ratio, ability to be engineered to respond to multiple stimuli and the compliance it offers to function under confined space make it a sought-after material kind for different engineering applications. In this talk, we will focus on two aspects - solvent responsive actuation and solvent-induced stiffening of biocompatible polymers and hydrogels. We will discuss how direction of actuation can be controlled along the entire spectrum of pH [1] for a bilayer based actuator. We will also focus on under-water and under-bath printing of biopolymers where separation-induced stiffening helps in 3D-printing of free-form structures which can be designed to actuate when exposed to different stimuli.

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RS-O1

Liquid crystal elastomer-based soft actuators

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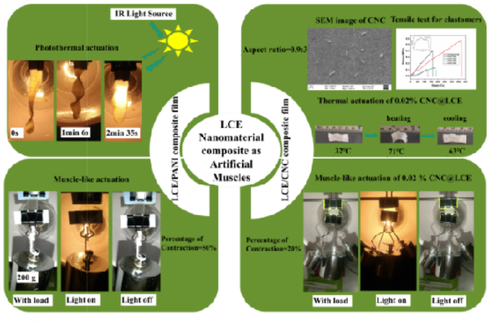
Soft actuation has gained tremendous research interest recently with a quest to create the nature mimicking soft, adaptive and collaborative electronic systems – soft robots and to develop artificial muscles. Liquid crystal elastomers (LCEs) are one such thermally driven soft actuators having unique properties namely, spontaneous reversible shape transformation with large actuation stroke, high processability and programmability[1]. Incorporation of nanoparticles (NPs) with interesting properties into the LCE matrix is one of the promising approaches for the easy manipulation of the actuating component in order to obtain a faster response and better control over the actuation.

In this regard, we have explored two different NPs in LCEs with a varied interest. Cellulose nanocrystals (CNCs) as ideal nanofillers in LCEs to improve the mechanical strength without compromising the elasticity and, polyaniline (PANI) NPs as photothermal agents to obtain a photoactuating system. LCE was prepared through a two stage thiol-ene Michael addition followed by photopolymerization. Different wt% of CNCs (0.01-0.05wt%, aspect ratio 0.3:1) were incorporated during the preparation of the elastomer to obtain the composites and influence of the CNCs on the mechanical and the actuation properties of the composite materials were studied. A composite film with 0.02 wt% of the CNCs displayed a maximum ultimate stress of 0.5MPa at an elongation strain of 372%. Interestingly, the films showed photoactuation in terms of contraction/elongation and weight lifting property. Similarly, the PANI NPs incorporated elastomers displayed various reversible actuations like contraction, rotation, twisting and widening on photoirradiation. Additionally, the composite films exhibited incredible weight lifting capability and one of the PANI (0.5 mg) doped film lifted a weight of 200 g, which is 1000 times of its own weight. The mechanical properties of these NP doped films are well above the min. standards (stress >0.35 MPa and the strain is >40 %) required for the artificial skeletal muscles and their actuation properties strongly pointed the suitability and potential of these composite films for the application as artificial muscles.



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RS-O3

Material Training through Mechanical Regularization

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Abstract: Training material through periodic drive enables materials to explore the high dimensional space of structures that exhibit complex elastic responses. However, increasing the complexity of the desired response results in ultra-slow convergence and degradation. Here, we show that by constraining the search space we can increase robustness, extend the maximal capacity, train responses that previously did not converge, and in some cases accelerate convergence by many orders of magnitude. We identify the geometrical constraints that prevent the formation of spurious low-frequency modes, which are responsible for failure. We argue that these constraints are analogous to regularization used in machine learning. Our results present a unified understanding of the relations between complexity, degradation, convergence, and robustness.

RS-O5

Tunable Textures in Cholesteric Liquid Crystal Shells for Sensing and Other Applications

Xu Ma, Yucen Han, Yan-Song Zhang, Yong Geng, Apala Majumdar*, Jan P.F.Lagerwall

Cholesteric liquid crystals are paradigm examples of mesophases, that are intermediate between the conventional solid and liquid phases of matter. Cholesteric liquid crystals are chiral and directionally ordered materials, with distinguished material directions referred to as “directors” and the cholesteric director naturally twists in space, adopting helical profiles. We study shells filled with prototype cholesteric liquid crystals, subject to different types of boundary conditions on the shell surfaces – tangential, normal and hybrid boundary conditions. We model these shells in the continuum Landau-de Gennes framework and numerically simulate equilibrium stable textures, as solutions of the associated Euler-Lagrange equations, which are a system of nonlinear partial differential equations. We demonstrate how the equilibrium structures respond to dynamic tuning of the boundary conditions, from textures with well-defined point defects on the shell surfaces o focal conics on the shell surfaces, as the boundary conditions are varied from tangential to normal. We compare our modelling results to physical experimental data on structural transitions in cholesteric shells, and they are in qualitative agreement. The rich library of optical textures of cholesteric shells with dynamically tunable boundary conditions opens new possibilities for photonic devices, thermal sensors, biosensors, and designer materials.

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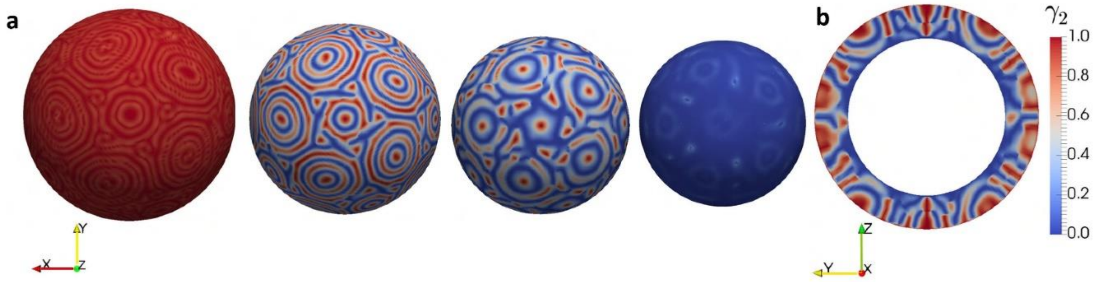

Understanding the role of polyproline's secondary structures in thermal phase transitions and bulk phase separations

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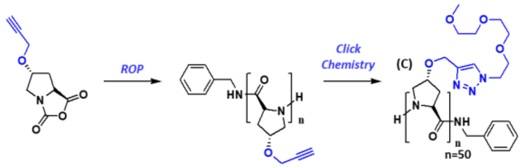
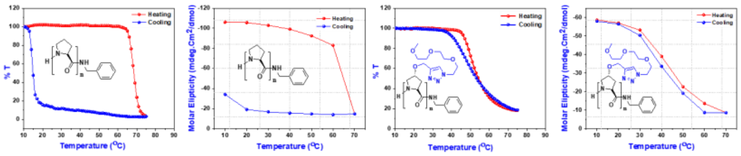
Abstract

Proteins are composed of amino acids, which play an essential role in their structure and functions. One of the 20 naturally occurring amino acids, proline, is the only one with a five-membered pyrrolidine ring attached to its side chain. Polyproline is unique among other polypeptides due to its cyclic side-chain and lack of an amide backbone that donates H-bonds. It is common for polypeptide backbones to assume -trans conformation, while polyproline can assume both -cis and -trans conformations. The conformation around the tertiary amide bonds in polyproline is crucial to the formation of their secondary structures. When the backbone amides are exclusively cis or trans, polyproline assumes a PPI (right-handed helix) or PPII (left-handed helix) secondary structure.[1] Different factors, such as temperature, solvent, substitution at C4-position, etc., can stabilize a particular secondary structure (PPI and PPII).[2]

In my presentation, I will describe a rational design of polyproline to stabilize PPI and PPII structures independently either via functionalization or copolymerization approach. Subsequently, I will explain how thermal phase transitions of polyprolines are related to their secondary structure.[3] Finally, I will discuss the role of polyproline's secondary structure during bulk phase separation of polyproline-based block copolymers.





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RS-O2

Reactive stimuli-responsive poly(aminoamide) microgels as a platform for diverse sensing applications

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Stimuli-responsive fluorescent nanomaterials are recently gaining a lot of attention due to their potential uses in diverse sensing applications.[1] In this regard, most of the reported materials suffers from their low water solubility, higher toxicity and lesser conformational stability for a range of applications.

Herein, we are reporting the synthesis of reactive, stimuli-responsive, biocompatible, fluorescent poly(aminoamides) microgels (NANO-PAMAM) as a platform for selective detection of temperature, pH and multiple metal ions. In the 1st part of the work, NANO-PAMAM is modified with doxorubicin (fluorescence acceptor) to build a ratiometric sensor for the detection of physiological temperature and pH.[2] In the 2nd part, a strategy is developed to prepare chitosan modified poly(aminoamide) microgels (NANO-PAMAM-CHT), for stimuli directed selective detection of multiple metal ions.

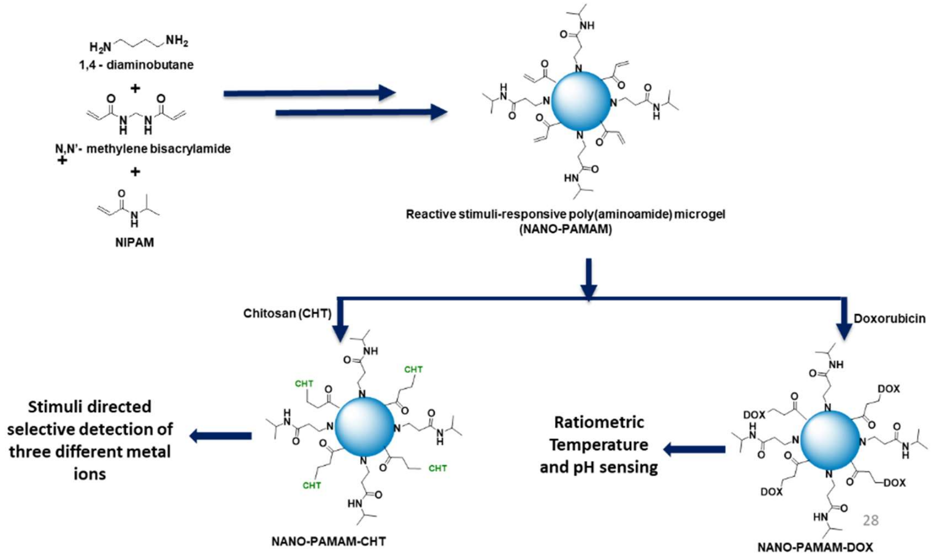

Figure 1: Synthesis and sensing applications of stimuli-responsive poly(amino-amide) microgels.

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RS-P1

A DPD study on the impact of external shear due to moving rigid walls, on the phase separation dynamics of polymer fluids

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ABSTRACT

This paper implements the Dissipative particle dynamics (DPD) simulation method to study the phase separation kinetics of critical and off-critical *AB* polymer blends. The system is induced by external shear arising due to the motion of rigid walls. Two amorphous solid walls are considered; one at the top, another at the bottom of the system. For the complete study, four different cases are explored: (i) Both walls are fixed, (ii) The top wall moves in positive *x*-direction while the bottom wall is fixed, (iii) Both walls move along the positive *x*-direction with same velocity, and (iv) Both walls move opposite in *x* -direction. An initial homogeneous mixture of the system is rapidly quenched to a temperature $T < Tc$, well below the critical value, and we monitor the effect of external shear on different properties like evolution morphology, scaling functions, domain growth, viscosity, etc. With the increase of shear rate applied to the system, polymer domains form a more ordered structure to overcome the external effect. The characteristic length scale follows the usual power law behavior; $R(t) \sim t^{\Phi}$, where Φ is the effective growth exponent. The expected macrophase separation is noted for both systems; initially, viscous hydrodynamic growth $\Phi \sim 1$ is followed, which crosses over to inertial hydrodynamic growth $\Phi \sim 2/3$ at the late time. Anisotropy is also developed in the system at a high shear rate due to the rearrangement of the domains parallel to the walls to get a more stable structure. For all cases, we noticed a decrease in viscosity with increasing shear rate representing the shear thinning in both systems. In the off-critical mixture, we observe some cylindrical *B*-type domains formed in case four at high shear rates, which is not noticed in other cases till this time interval.

KEYWORDS

DPD Simulation, Polymer Blends, Growth Laws, Anisotropy.

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Preparing functional soft materials through the directed self-assembly of complex liquid crystals

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Liquid crystals (LCs) combine the structural anisotropy of crystalline solids with the fluidity of liquids. While controlling the structure of simple liquid crystalline phases, such as nematics is well-understood, alignment of complex liquid crystals such as blue-phases and discotics is more challenging. We present here two methods to align complex liquid crystalline phases, namely chemo- and grapho-epitaxy. These techniques involve making chemical and topographical patterns using nanolithography. Chemo and grapho-epitaxy are well established techniques in the field of block copolymers. We present here extensions of these techniques for assembly of liquid crystalline phases. We demonstrate how directed self-assembly of blue-phase and discotic liquid crystals can be used to prepare polymeric photonic single crystals[1,2] and biaxially textured crystals of organic semiconductors[3], respectively.

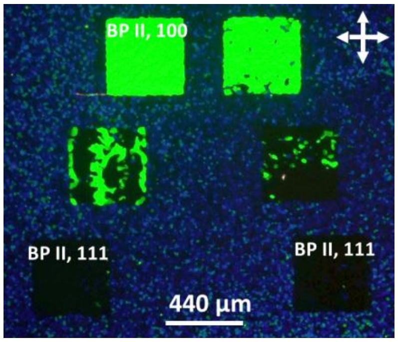

Figure 1: Green and UV-reflecting single photonic crystals created through directed self-assembly of blue phase liquid crystals. The squares regions are patterned regions.

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RS-P3

Topological defects and electrokinetics of emulsion droplets in nematic liquid crystals

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We describe the preparation and characterization of different shapes of emulsion microdroplets e.g., Janus and Snowman type in nematic liquid crystals (NLC) and studied their topological defects mediated self-assembly and transport by the application of external alternating electric field through the mechanism of liquid crystals enabled electrophoresis (LCEP). We measure the propulsion speed of these emulsion droplets in NLC, based upon the parameters like droplet's shape, size, defects, and the strength and frequency of the applied electric field. We prepare different LCs based Janus droplets in water based medium also and analyse their morphology with varying surfactant concentration and volume ratio of LCs and polymer. LC based Janus droplets with remarkable optical properties and controlled transport provide challenging applications in controlled assembly, sensing, targeted delivery and optical resonace.

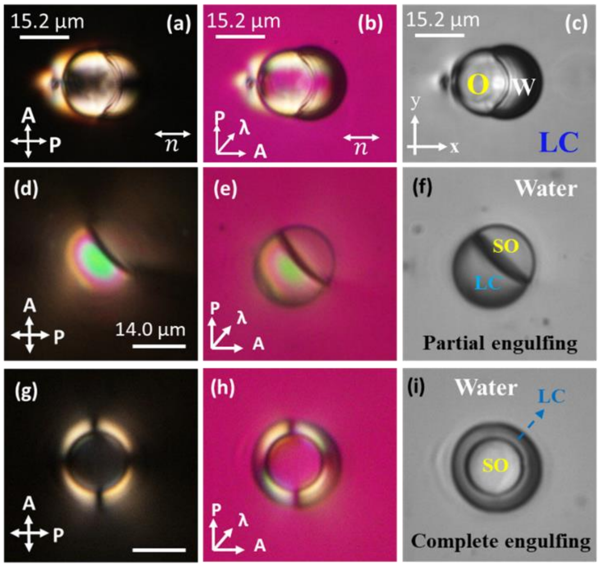

Figure 1: Polarizing optical microscope (POM) images of emulsion droplets with different morphologies. (a)-(c) are images of Janus droplets in NLC, (d)-(i) are images of Janus droplets in water based med. (a),(d),(g) are cross polarized images, (b),(e),(h) are corresponding images of same droplets taken by inserting a λ plate (530 nm) with slow axis at an angle of 45° between the sample and analyzer. (c),(f),(i) are the corresponding ccd images. Double headed arrow represents the nematic director. *P*, *A* represents polarizer and analyzer.

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Hot crystals of thermo-responsive particles with temperature dependent diameter in the presence of a temperature gradient

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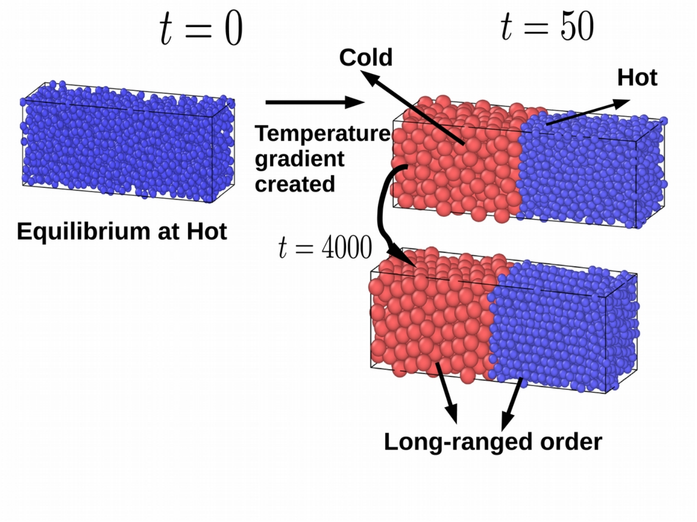
Abstract

Structure formation in non-equilibrium steady state conditions is poorly understood. Non-equilibrium steady state can be achieved in a system by maintaining temperature gradient.

PNIPAAM, a cross-linked micro-gel particles, are reported to increase in size due to absorption of water with decrease in temperature. These thermo-responsive particles are experimentally reported to form aggregates in cold region of the system in presence of temperature gradient. Here we model the system as particles with temperature sensitive diameter, using Molecular dynamics simulation with Langevin thermostat as per the local temperature. We find long-ranged structural order using bond order parameters in both cold and hot region of the system beyond a certain diameter ratio of the cold and hot particles. The intriguing phenomenon of ordering in the hot region is due to increase in packing and the overall steady state pressure. Our model [1] illustrates a simple case where high temperature crystallization can be studied in the laboratory and provide insight to mechanism of formation of long-ranged order in extreme condition in steady state.



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Indian Society of Rheology

RS-P5

Nucleation of Bulk Nanobubbles During Oscillating Pressure Field

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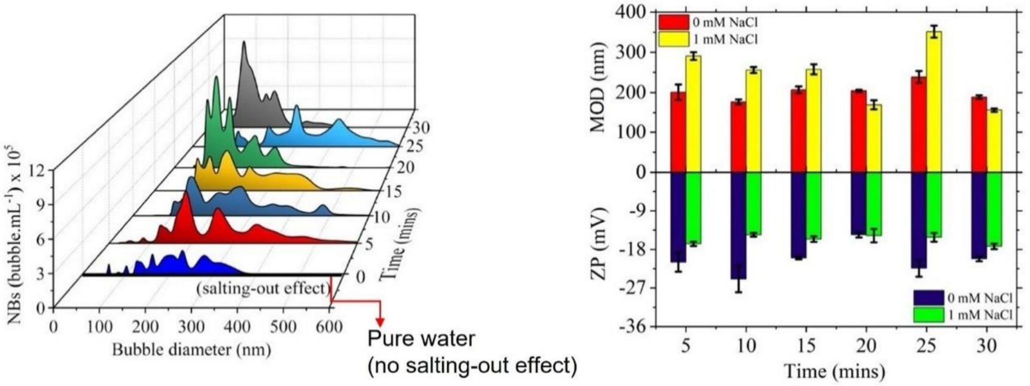
Nanobubbles are nanoscale bubble swarms with several peculiar properties that have been demonstrated to have a widespread application [1,2]. In view of long-term stability [3], bulk nanobubbles picked up additional interest over the years. The influence of an oscillating pressure field on nanobubble dynamics during salting-out enhances the bubble number density. The refractive index calculation and the electrical conductivity confirmed the evidence for the gas-filed nanobubbles. The screening of the electric double layer decreases the surface potential depending on the valency of the salt. Therefore, the equilibrium size of nanobubbles was observed to be higher in the presence of salts. The mean diameter of these bubbles exhibits an inverse dependence on the surface potential, owing to the clustering effects of nanobubbles.



(a) (b)

Figure 1: Bubble dynamics during pressure disturbance (a) Bubble size distribution (b) Mean diameter and zeta potential.

Figure 1a depicts the temporal development of the nanobubble size distribution in pure water and 1 mM NaCl solution, where the bubble distribution area grows with cycle time and the surface charge directly relates to the mean diameter gained by these gaseous cavities (see Figure 1b).

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Transport of magnetodielectric particle in a nematic liquid crystal under transverse electromagnetic fields

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Synthesis of micro and nanoparticles of pre-designed shape and surface properties is integral to soft and synthetic active matter [1]. We fabricate matchstick-shaped (MS) magneto-dielectric particles and explore their potential as active particles with field-controllable trajectories in a nematic liquid crystal (NLC). The MS particles with homeotropic anchoring in NLCs nucleate either point or ring defects consequently they align either parallel or perpendicular to the director. When subjected to transverse electric and magnetic fields, the particles experience electric and magnetic torques trying to align them in the respective field directions. At equilibrium, the long axis is tilted at an angle with respect to the director. The change in orientation alters surrounding elastic distortions which result in unbalanced electro-osmotic flows in two orthogonal planes. These flows provide the necessary impetus for propelling the particles in various directions with different velocities depending on their orientations.

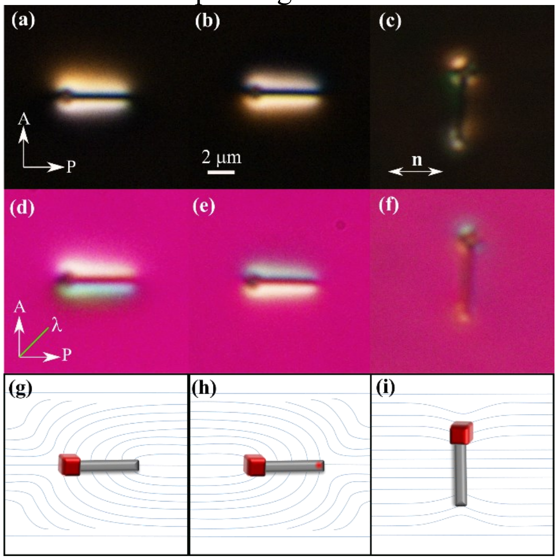

Figure 1: POM images of DMOAP coated matchstick particles in ZLI-2293 with (a) a point defect at the side of the cube, (b) a point defect at the tail-end, (c) a ring defect through the long-axis of the particle, (d-f) corresponding red plate images obtained by inserting a full wave plate at 45° between the crossed polarisers, and (g-i) schematic of the director profiles. P, A represents the polariser and analyser. White double-headed arrow denotes the director.

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RS-P7

Ethylene glycol energetically destabilizes aggregates of pseudoisocyanine dyestuffs at crowded concentrations

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Abstract

The structural changes of the proteins within the complex and crowded cellular environment is still remains elusive.[1] The “soft-interactions” are essential for governing the stability of test proteins, which are widely recognized for their significance within the cellular environment.[2,3] As a result, the influence of attractive or repulsive interactions has the potential to counterbalance or overcome the destabilizing impact caused by the excluded volume effect of the crowding agents on the test proteins.[4] In our research, we have investigated the aggregation behaviour of pseudoisocyanine chloride (PIC) dyestuff, which is recognized for its tendency to form-fibril like structures called J-aggregates.[5,6,7] These J-aggregates bear resemblance to the amyloid formations observed in proteins known to exhibit amyloidogenic behaviour.[8] According to previous studies, ficoll-400 promotes the self-assembly of PIC-dyes, whereas polyethylene glycol hinders their self-assembly.[9,10] In order to gain the deeper insight, we employed the enhanced molecular dynamics simulations to investigate how the presence of aqueous ethylene glycol affects the solvation thermodynamics of PIC dyes capable of forming H- and J-types oligomers. Our finding have provided deeper comprehension of free-energy calculation, revealing that in pure water, J-oligomers exhibit greater stability compared to the formation of H-oligomers. In pure water, the tetramer of H-oligomers exhibited the highest stability while J-oligomers stability increases as the oligomer size increases. However, the H-oligomers become less favourable in ethylene glycol, and the formation of tetramer and pentamer is also favourable for J-oligomers. Moreover, the formation of oligomers is driven by the favourable change in the interaction energy of dye-solvent upon PIC association, observed in both pure water and aqueous ethylene glycol solutions. However, this inclination is mitigated by the reduced entropy of the dye-solvent system, imposing a restraint on oligomer formation. Moreover, the presence of ethylene glycol crowders induces the destabilization of H- and J-type oligomers by exhibiting preferential binding to the dye-oligomers. Our findings aligns with the experimental observations (Isothermal Titration Calorimetry) from a previous study, wherein it was demonstrated that TEG and PEG impede the aggregation of dyes.[11], Thus, it can be inferred that a molecularly crowded environment tends to disfavour the self-assembly of the PIC dyes by engaging in interactions with the oligomers rather than promoting self-assembly within (bio)molecules.

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Controlled actuation of gelatin based soft actuators in response to multiple vapor

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Soft actuators represent a highly promising and transformative approach to revolutionizing robotics and automation, particularly in domains like medical technology and human-robot interaction. Attributes such as rapid and reversible actuation, biocompatibility, and precise control over actuation magnitude and direction are imperative for their seamless integration into modern technological landscapes. However, the current employment of synthetic polymers and nanomaterials in soft actuator design is constrained by issues such as elevated costs, lack of biodegradability, and intricate synthesis procedures.

Here we report, a bio-polymer-based, bio-compatible, single-layer gelatin-based soft actuator with responsiveness to multiple vapors. This novel actuator exhibits swift, reversible, and repeatable actuation across more than 1000 cycles. Moreover, it display distinct reactions to water and ethanol vapors. By manipulating the bending axis via surface patterning of the gelatin film, precise command over actuation magnitude and direction is achieved. Notably, the patterning of the gelatin film's surface facilitates a transformation from random locomotion to linear motion.

We also demonstrate, promising applications of gelatin-based soft actuator in ethanol-vapor sensing, intelligent curtains, automated lifts, adaptable wearable textiles, and bio-mimetic systems. Leveraging the actuator's biodegradable nature and cost-effective fabrication process opens up novel avenues for practical implementation across robotics, biomedical devices, and diverse fields necessitating compliant and versatile motion.

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RS-P11

Vapor-responsive tunable actuation of silk films: Effect of secondary structures

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Precise coordination of the expansion and contraction of soft tissues within living organisms, both in terms of space and time, give rise to distinctive shapes and even enable locomotion. However, replicating these intricate natural motions within a controlled laboratory environment remains a formidable task. To overcome this challenge, adaptable soft materials responsive to a range of stimuli, including vapour, electric fields, temperature, and light, are being actively explored. These materials find utility, especially in environments that are typically hard to access using conventional technologies. Notably, the flexibility and compliance of soft actuators allow them to navigate complex and dynamic surroundings seamlessly, rendering them ideal for manipulating fragile objects and operating within confined spaces.

Of particular interest are biopolymer-based vapour-responsive soft actuators, as they possess a distinct advantage over alternative soft materials due to their innate biocompatibility and biodegradability. One such biopolymer, *Bombyx mori* silk fibres, referred to as fibroins, stands out due to their exceptional and wide-ranging properties such as high strength, lustre, slow degradation, abundance, and ease of processing. Notably, these protein-based silk fibres exhibit secondary structures, specifically *alpha* and *beta* configurations, which influence not only the properties such as strength and stiffness but also the water sorption capacity, which makes them ideal candidates for designing tuneable water vapour-responsive soft actuators. Moreover, the manipulation of these secondary structures via water vapour annealing or by other means makes the silk fibroins even more suitable for achieving tunable actuation. Consequently, we demonstrate that the speed and extent of actuation can be finely tailored by simply modulating the proportion of the distinct phases in silk films. The vapour-responsive large-scale locomotion of silk fibroin films, along with the physics of the actuation process, will be presented in detail.

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Abstract Title

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Twist-bend (N_{tb}) and ferroelectric (N_F) nematic liquid crystals exhibit several novel effects and new physical properties. The question of what happens in binary mixtures is interesting as a matter of curiosity and pure science. Here, we report experimental studies on the phase diagram and some physical properties of binary mixtures of the above-mentioned nematic liquid crystals. Both N-N_{tb} and N-N_F phase transition temperatures and the corresponding enthalpies decrease significantly and eventually, these transitions disappear in some intermediate compositions. Temperature-dependent birefringence above the N-N_{tb} phase transition temperature shows critical behaviour, and the critical range of the tilt fluctuations becomes wider in the mixtures. The magnitudes and the temperature dependence of the splay elastic constant of the mixtures' high-temperature nematic (N) phase strikingly differ from that of the pristine twist-bend and ferroelectric nematic liquid crystals. The study shows that N_{tb} and N_F liquid crystals are incompatible.

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Understanding The Role Of Shape-Dependent Anisotropy Of Electrostatically Driven Nanoparticle Self-Assembly

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Nanoparticles (NPs) with facile surface chemistry and unique optoelectronic properties have shown tremendous interest in biology and nanomedicine, especially for cancer cell imaging, cellular targeting, pharmacokinetics, and biodistribution[1]. The increased potential of nanoparticles for applications has moved them from basic research, majorly driven by scientific curiosity, into the focus of technological interest[2]. Recent findings have shown that particle shape is an important design parameter that considerably influences their potential in biological applications. Recent studies on metallic nanoparticles showed that particles of different shapes, such as rods, triangle-like, hexagonal, cubic, octahedral, tripod, star, and tetrapod, were synthesized. Controlling the assemblies of these nonspherical nanoparticles. With the increased precision of functionalizing polymeric ligands on nanoparticles using concepts of click-chemistry, nanoassemblies of greater complexity and sophistication can be obtained. In this work, molecular dynamics simulations are performed to understand the transitions in assemblies of polyion-grafted nanoparticles (PGNs) of different 2D shapes, including nanorods, nanotriangles, nano squares, nano tetrapods, and nano polygons. By varying the graft length and graft chain stiffness, precise control of morphological transitions was achieved. The obtained morphologies were analyzed to explain the role of particle geometry on the thus-formed morphologies.

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Coupled Photo-Mechanics of Nematic Liquid Crystal Elastomers - An ABAQUS UEL Implementation

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Light-responsive liquid crystal elastomers (LCEs) have been at the forefront of stimuli-responsive actuators in the recent past. The light-responsive elastomers are created by doping the elastomeric network with the azo-benzene mesogens. The elastomeric network's weak cross-linking and the mesogens order-disorder transition lead to certain exotic behaviors, as mentioned below.

1. The stretching of poly-domain LCEs results in the uni-axial alignment of the mesogens.
2. The rise in temperature leads to Nematic-Isotropic transitions and large deformations.
3. The weak cross-linking of the elastomers coupled with *trans-cis* isomerization of the azo-benzene leads to changes in the alignment of the elastomer resulting in large mechanical deformations upon illumination (Photo-mechanical coupling).

In this study, we have developed a user element subroutine (UEL) that simulates the photomechanical coupling of these nematic elastomers under mechanical stress and illumination using the commercial finite element software Abaqus. To model the photomechanical coupling using the finite element method, the minimization of the free energy approach is implemented considering Corbett and Warner's formulation [1] for polymeric network elastic behavior and Maier-Saupe theory-based formulation [2] for nematic liquid crystal behavior. A system of linear equations with displacements, order-parameter and the alignment direction as primary variables is developed following the Rayleigh-Ritz and Newton-Raphson method. The developed model is benchmarked by comparing the output of a 2D LCE sheet with the work of Bai and Bhattacharya [2]. Additionally, the created UEL is then used to simulate the unusual behaviors of the LCE sheets that were previously discussed. The developed framework can also be expanded to simulate the coupled photomechanical response of LCEs with patterned alignment distributions.

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Effect of Counterions on Polyelectrolytes: A Molecular Dynamics Simulation Study

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The studies on Polyelectrolytes provides classical insights on broad range of materials. Common examples of Polyelectrolytes are the DNA and the RNA. Molecular Simulation studies reveal the molecular-scale behavior that provides the structure-dynamics of various property relationships. It generally uses the common bead-spring models for performing the molecular dynamics simulations of Charged Polymers. These models show great abilities in studying the polymer properties such as polymer phase behavior as a function of temperature. Simulations can do much better in terms of accuracy compared to experimental setup. We represent the monomers in the form of beads attached through a spring. This spring has a spring constant with k=7∈/σ^2. All monomers are bonded through the FENE (Finitely-Extensible Non-Linear Elastic) bond. Further, in addition to that we introduce counterions to the system to neutralize the charges. Hence, our system is then placed inside a cubic box. To study the dynamics of the system the system is equilibrated to certain time duration to attain the equilibrium conditions. Then we perform the calculations such as the radius of gyration, mean squared displacement, end-to-end distance, and radial distribution function. With this study, we are going to determine the phase transition from the coacervate phase to single phase and plot the Phase diagram. In addition to this, we also explore the formation of Liquid-Liquid Phase separation and then evaluate the density profiles of polymers and free ions.

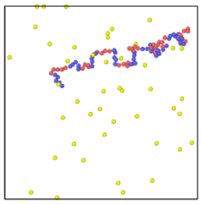

Figure 1: Flexible polyelectrolyte

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Role of interfacial properties on the mechanical deformation in light-activated polymer blends

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Light-activated polymers (LAPs) have been known for their unique ability to "shape-shift", in response to light exposure that serves as an instant and precisely controllable non-contact stimulus. One of the key mechanisms to induce shape changes in LAPs is the *cis-trans* isomeric transformation stimulated by light as shown in Fig.1(a). Although blending has emerged as an effective route to synthesize LAP blends (LAPBs) and other shape memory polymer blends (SMPBs), tailoring their mechanical behavior still remains a grand challenge. Primarily, the immiscibility between constituents results in poor interface strength, between polymeric domains, which leads to inferior mechanical properties of LAPBs and SMPBs. The overall objective of this work is to establish design rules, via modelling and simulations, by coupling the phase and mechanical behaviours of LAPBs. To this end, we develop a unified framework that captures the effect of interfacial properties emanating from phase separation on mechanical deformation in polymer blends under isothermal conditions. To establish the mechanical behaviour, we harness the free energy approach and develop a non-linear constitutive model wherein the composition-dependent mechanical properties of the blend are predicted from the individual properties of the components. Our study reveals that, apart from the mechanical properties of individual polymers, the interfacial stress between phase-separated domains is directly related to interfacial tension. From a practical standpoint, therefore, the mechanical response of LAPBs can be tuned by adjusting the surface energy densities at the interface of phase-separated domains. The advantage of our approach is that it does not only provide an efficient pathway to design multi-component polymer blends or LAPBs with tailored properties but can also be harnessed to capture the structure-property relationships for shape memory polymer blends.

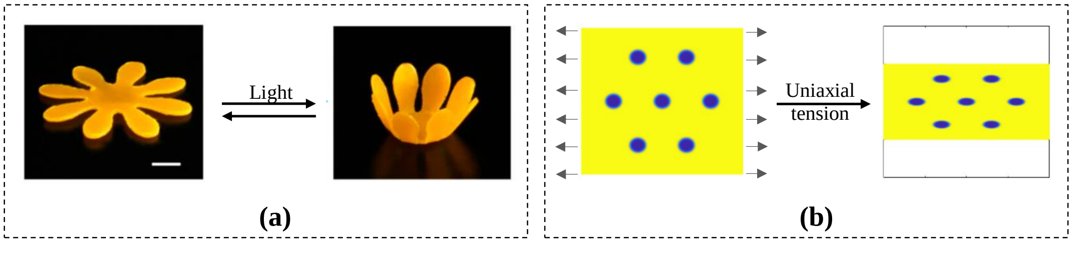

Figure 1: (a) Shape changes in light-activated polymer blend due to *cis-trans* transformation on light irradiation. (b) Deformation in polymer blend with droplet matrix morphology under uniaxial tension.

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Multi-dye-based light/thermal responsive liquid crystal polymer films

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Liquid crystal polymers (LCPs) are formed by the polymerization of reactive mesogens. The average direction of the major axes of ellipsoidal shaped liquid crystal molecules is the director orientation. When subjected to heat there will be contraction along the director direction and expansion in perpendicular direction. This produces a through thickness strain gradient and reversible actuation. These polymers with lower cross link density are liquid crystal elastomers (LCEs) and with higher cross link density are liquid crystal glassy networks (LCNs). The LCPs can be made photo responsive by doping with photosensitive dyes. These dyes have maximum absorbance at certain wavelength (λ_{max}) and gives maximum actuation at those peaks. Soft robotic actuators based on LCPs responsive to multiple wavelengths were made using bilayer and trilayer films [1]. But the possibility of getting broader wavelength response by doping with multiple dyes in same film is yet to be explored.

In this work, we have prepared twisted nematic thin films of LCNs with two different dyes namely A3MA ($\lambda_{max} = 365$nm) and DR1A ($\lambda_{max} = 483$nm). The absorbance spectrum of multi-dye films shown two peaks corresponding to the λ_{max} of doped dyes. DR1A dye converts the light to heat whereas A3MA introduces one more phenomenon of network pull. The actuation response of multi dye films was studied and compared with films having a single dye and also bare LCN film without any dye to understand the influence of multiple dyes in a single film. A computational model was prepared in ABAQUS to simulate the actuation. It was observed that the addition of more than one dye broadens wavelength response and hence range of actuation.

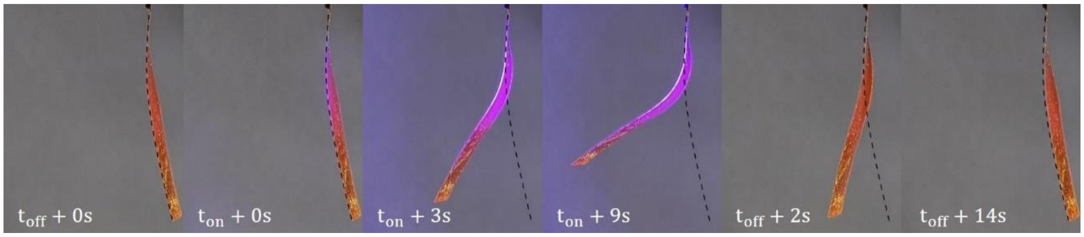

Figure 1: The actuation of LCN film with A3MA & DR1A dye, having twisted nematic alignment when subjected to 455nm light. The dotted black line shows the initial position of the film.

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"Numerical Investigation of Coupled Swelling-Deformation Behavior of Functionally Graded Hydrogel Thin Films"

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Hydrogels shows stimuli-responsive behavior upon exposure to an external environment like temperature, pH, solvent etc. The hydrogel films discussed in this presentation undergo shape morphing in the presence of water. To achieve shape change under different environmental conditions layered materials with different material properties are preferred. But the layered films limit the functionality to a great extent because of the uneven force distribution at the interface. Hence, the use of a mono-component functionally graded film(FG) is proposed. The actuation of FG film in presence of water is modeled using a coupled diffusion deformation formulation based on Flory-Huggins theory [1]. It considers the change in free energy due to the mixing of the water molecule with the polymeric network. Owing to the similarities between the diffusion and heat transfer equations, the inbuilt ABAQUS coupled temperature-displacement is employed to simulate the swelling-induced deformation of polymer thin film [2]. Finally, the results from the finite element (FE) model are corroborated with the experimental results for a chitosan-water system by comparing the folding path and curvature. The developed model can aid in developing and designing new material models for targeted applications.

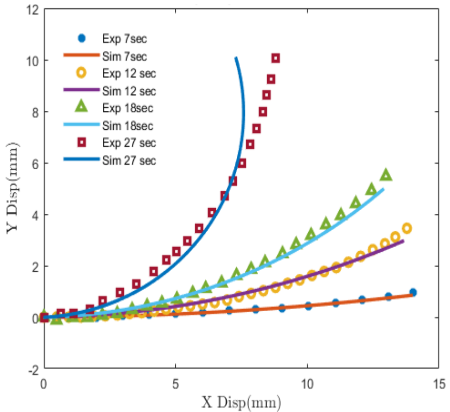

Figure 1: Time stamps for the out of plane displacement of FG film for experiment and simulation .

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Indian Society of Rheology

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Computational validation of stimulus-responsive anisotropic PVDF film

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Poly(vinylidene fluoride) (PVDF) is a versatile semi-crystalline fluoropolymer chain responsive to organic vapors. This report proposes a fast-responsive unilayer thin PVDF film composed of α and β phases. The ratio of these phases varies with the drying temperature during film preparation, resulting in an anisotropic distribution. The α phase has a stronger affinity for the stimulus (acetone) than the β phase, resulting in unequal swelling [1]. Films prepared at different temperatures were studied for their response rates, with the fastest being less than 0.5 seconds.

Computational simulations of the actuation process were carried out using ABAQUS CAE. Since no built-in model for vapor deformation is available in ABAQUS, we exploited the similarity between the general governing equations of vapor absorption and heat transfer to use the built-in coupled-temperature displacement model to mimic the actuation process. Phase variation data from FTIR spectroscopy was used to assign anisotropic material distribution. User-subroutines were used to tailor the acetone boundary condition in real-time. The mechanical aspects of the actuation behavior were studied, and the simulation results were in good agreement with the experimental results.

This study showcases PVDF films' potential for rapid soft actuation. Control over α and β phase distribution, influenced by drying temperature, enables actuation response tuning. Computational simulations contribute to comprehending the film's actuation process and mechanical traits.

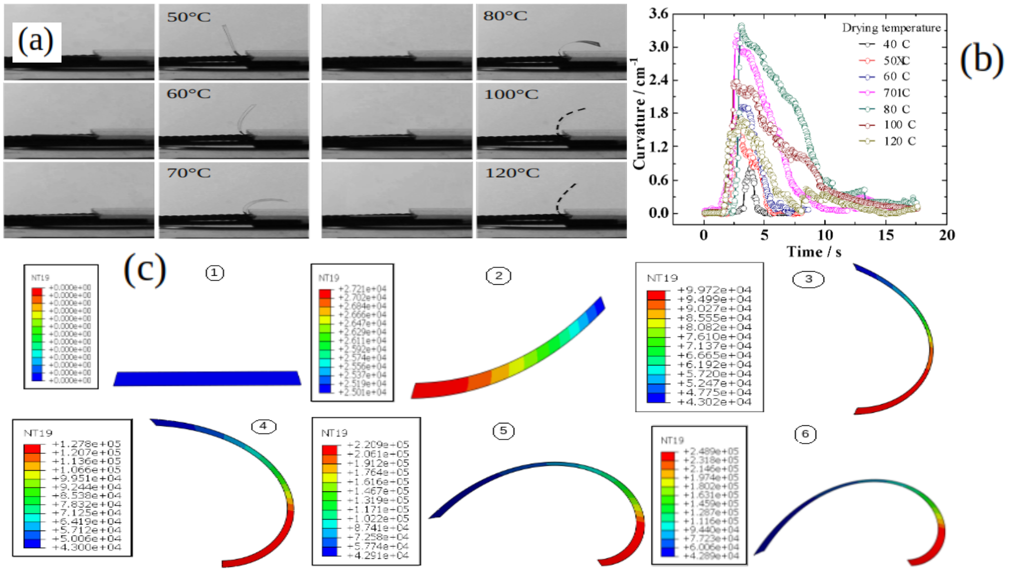

Figure 1:(a) actuation of PVDF film formed at different drying temperatures, (b) Bending Curvature Vs. Time graph, (c) Simulation of PVDF film formed at 80°C

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RS-P20

Buoyancy-driven microgel oscillator: Beating and Bouncing dynamics.

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Chemo-mechanical oscillators, drawing inspiration from biological dynamics, provide a fascinating platform to unravel the intricate interplay between chemical reactions and mechanical motion. In this context, diverse designs have been explored, including those within homogeneous [1,2] and stratified media.[3] In our study, we introduce a novel chemo-mechanical oscillator design in a stratified three-layer particle-based density medium utilizing ion-specific responsiveness of Ca^{2+}-alginate /chitosan microcapsules. Ca^{2+}-alginate/chitosan microcapsules exhibit tailored swelling and deswelling responses that oscillate between the top and bottom density interfaces of antagonistic layers. Buoyancy force serves as a driving mechanism, fueling the dynamic interactions within this stratified media, ultimately manifesting in versatile and controlled chemo-mechanical oscillations. The capsule density relative to the middle layer influences oscillation behavior, resulting in sustained or damped oscillations. This behavior is explained by the density-based excitation theory. Our study presents the remarkable synergy between chemical reactivity and buoyancy-driven motility, highlighting how this coupling can lead to emergent behaviors within stratified media.

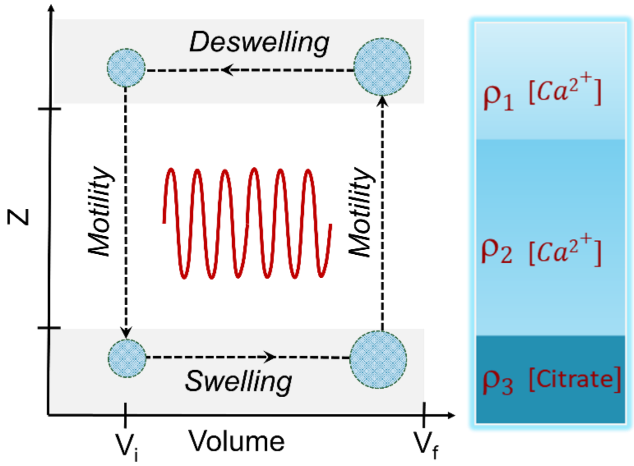

Figure 1: Schematic of buoyancy-regulating chemo-mechanical oscillation in Ca^{2+}-alginate/chitosan microcapsule (left) in a stratified density gradient(right).

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RS-P21

Studying the effect on yielding behaviour of dense suspensions of thermo-responsive PNIPAM particles by tuning inter-particle interactions

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PNIPAMs are well known microgel particles which undergo a reversible volume phase transition from being hydrophilic to hydrophobic with increase in temperature above a critical value known as LCST [1]. In an aqueous environment, dense suspensions of PNIPAM particles are known to go from being repulsive glass to colloidal gel via a liquid like phase with increase in temperature [2]. We use dynamic light scattering and rheology to study the modification in their inter-particle interaction by systematically adding salt into the suspension. At low applied shear (linear viscoelastic region) it is seen that below LCST the elastic modulus of the suspensions goes down with increase in salt concentration. Above LCST there is a crossover from viscoelastic solid to viscoelastic liquid where the crossover frequency decreases with increasing salt concentration. Under high applied shear (non- linear regime) the suspensions show single step yielding below LCST with the yield strain decreasing with increase in salt concentration. Above LCST though, the system displays two-step yielding typifying colloidal gel like/attractive glassy behavior. Strain separation between the two yield strains (1st yield point and 2nd yield point) coming from this two-step yielding decreases with increase in salt concentration. This indicate towards an increase in attractive strength with increase in salt concentration [3].

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Novel composite hydrogels with enhanced thermal stability and injectability

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Interactions between the colloidal particles and the amphiphilic species play a major role in determining the overall microstructure of the composite systems. The effect of the addition of hematite pseudocubes/ akaganeite (β-FeOOH) nanorods in PF127 triblock copolymer solutions on the viscoelastic behavior, elastic strength, mechanical fragility, thermal stability, enhanced injectability etc., of the composite gel is studied through linear and nonlinear rheological behavior of this composite system. Even at small concentrations, the presence of β-FeOOH NRs can modify the strength and flexibility of PF127 gels. External magnetic field is used to tune and control the chain-like microstructures of hematite cubes in the composite gels. These gels show thermoresponsiveness and enhanced injectability, and could find applications in tissue engineering and drug delivery.

Figure 1: Composite hydrogels containing small amounts of paramagnetic akaganeite (β-FeOOH) nanorods in PF127 triblock copolymer show enhanced thermal stability and injectability which could find applications in tissue engineering and drug delivery.

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Role of finite extensibility on the center-mode instability in viscoelastic channel flow

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A linear center-mode instability was recently reported for plane Poiseuille flow of ultra-dilute (solvent to solution viscosity ratio $\beta \geq 0.99$) highly elastic (Weissenberg number $W \sim 1000$) polymer solutions within the framework of the Oldroyd-B model [1]. This prediction defies the conventional paradigm that requires hoop stresses as a necessary ingredient for purely elastic instabilities. Subsequently, it has been shown [2], using the FENE-P (finitely extensible non-linear elastic spring with Peterlin closure) model, that the instability persists down to W of O(100), pointing to the rather counter intuitive destabilizing role of finite extensibility of polymer molecules.

In this work, we augment the latter finding above, by providing a comprehensive account of the role of finite extensibility on the center-mode instability in viscoelastic channel flow, using the FENE-P and FENE-CR (Chilcott-Rallison) models, both in the absence and presence of fluid inertia. In general, finite extensibility causes a decrease in the polymer relaxation time at high shear rates, and consequently, is expected to have a stabilizing effect, an expectation that is borne out in the context of hoop-stress driven instability in curvilinear shearing flows. This is indeed the case for the FENE-CR model, where finite extensibility largely shows a stabilizing effect on the original center-mode instability. In stark contrast, for the FENE-P model, we show that finite extensibility plays a dual role – stabilizing at lower values of the elasticity number E (= W/Re), but destabilizing at higher E's. Furthermore, the center-mode instability for the FENE-P model is predicted over a larger domain in the Re-E-β parameter space, compared to the Oldroyd-B model. All of these factors make the center mode instability potentially more amenable to observation in realistic parameter regimes.

Acknowledgements: Mohammad Khalid, Debanjan Dutta, Amit Badoni, and Prajwal Naidu (IIT Kanpur).

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The linear and nonlinear rheological characteristics of the biofilm formed by Mycobacterium Smegmatis.

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Aggregated bacterial colonies organized inside an extracellular matrix (ECM) are called biofilms. The biofilm's architecture is governed by the ECM, which also provides mechanical resistance to shear pressures. The study shows deformation and flow, focuses on how small- and large-scale interactions within the structures of materials affect the mechanical behavior at various scales. To understanding how biological function, physical structure, and chemical circumstances interact to determine biofilm rheology thus requires an understanding of the structure-function interactions that govern biofilm rheology and define the mechanical properties of a biofilm. For macroscale investigation of biofilms, we use of rotating oscillatory shear tests, stress relaxation tests, rheometers enable direct assessment of viscoelastic material properties. In our experiment we are using Ex situ growth on agar plates and transferred to the rheometer. To determine the elastic and viscous responses of the material using equations presented by Ferry. The parameters typically referred to as the elastic modulus (G′) and loss modulus (G″) characterize the material's stiffness and fluidity, respectively. In order to calculate the elastic and loss moduli, it is necessary to assume that the material is under infinitesimal strain and that the input and output waveforms are sinusoidal. When performing an amplitude sweep measurement, the material is exposed to sinusoidal strain waveforms of increasing amplitude while the oscillation frequency remains constant. A typical amplitude sweep result for biofilms is shown in the figure1. At low strain amplitudes, the elastic and viscous moduli show constant values; this regime is known as the linear viscoelastic region (LVER). The strain and stress signals in the LVER continue to be sinusoidal, indicating the material's linear reaction. Due to the application of minimal strain the material structure is fully unaltered. Beyond the LVER, the stress waveform is no longer sinusoidal at higher strain values. Depending on the size of the input strain, local stiffening/softening or yielding of the material may take place in this nonlinear area, where polymer entanglements breakdown and material structure is rearranged. It describes the nonlinear rheological behavior occurring inside the materials.

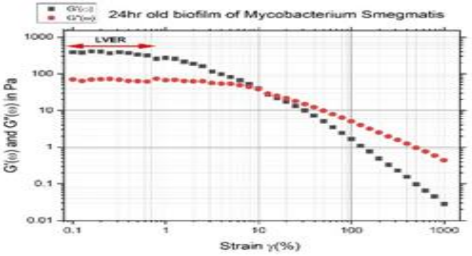

Figure 1: Amplitude sweep showing the variation of G′ and G″ as a function of strain.

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Tuning the non-linear rheological response of low molecular weight supramolecular gels

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Supramolecular 3D hydrogels represent a class of materials, characterized by the self-assembly of low molecular compounds (which act as gelators) leading to a 3-D network. The resulting gel structure is held together by weaker reversible interactions such as hydrogen bonding, vander Waals forces and π-π interactions. This allows for precise tuning of the physical, chemical and mechanical properties of the gels. This endows numerous design possibilities of these gels thus making them promising candidates across diverse applications. Considering these design possibilities and applications, rheological characterization of these gels is of great interest. Functionalized Fluoromethoxycarbonyl (FMOC) is considered as a minimalistic model for low-molecular weight gelator. The physical interactions and the overall properties of these gels can be varied by varying the functional group in the gelator. Supramolecular gels with distinct functional groups i.e. FMOC-β-Phenylanalaine, FMOC-L-Tyrosine and FMOC-Phenylanaline are characterized using large amplitude oscillatory shear rheology (LAOS). The distinct non-linear rheological characteristics of these gels are compared and the influence of physical interactions on their rheological properties is also studied. Insights from this study will help in better optimization of these gels for targeted applications.

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A unified state diagram for the yielding transition of soft colloids

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Concentrated colloidal suspensions and emulsions are a prototypical example of amorphous soft solids, widespread in technological and industrial applications and intensively studied as model systems in physics and material sciences. Soft solids are easily fluidized by applying a mechanical stress. Although the yielding transition has been actively investigated, no consensus on a unified description has emerged so far.

Here [1], we investigate yielding in three classes of soft solids, using analytical and numerical modelling and experiments probing simultaneously the microscopic dynamics and mechanical response under oscillatory shear. We find that at the microscopic level yielding consists in a transition, sharper than for rheological quantities, between two distinct dynamical states. We propose a lattice model with dynamical coupling between neighboring sites that captures the generic features of our experiments, leading to a unified state diagram for yielding. Disorder in the dynamical coupling plays a major role in the emergence of first-order-like vs second-order-like features in yielding, allowing for reconciling previous contrasting observations on the nature of the transition.

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Fractional calculus derived empirical predictive relations for the linear viscoelasticity of semi-dilute polymer solutions

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The oscillatory viscoelastic functions of polymer solutions often exhibit a power-law response, of the form $G'(\omega) \sim \omega^{\alpha}$ which are not well modeled using canonical generalized Maxwell modes. Recently, there has been a strong revival in applying fractional order constitutive modes for studying the response of a variety of complex fluids. Here, using poly(ethylene) oxide (PEO) in water as a model system and Bayesian statistics, we demonstrate that modeling their frequency-dependent complex moduli entails upwards of 20-Maxwell modes whereas, an equivalent good-fit is obtained using a single mode fractional equivalent. This greatly reduces the dimensionality of the model parameters from $\in R^{\sim 40}$ to $\in R^{\sim 4}$. Furthermore, we study the $c - M_w$ dependence of the fractional model parameters and discuss an empirical relation for predicting different linear viscoelastic functions of semi-dilute aqueous solutions of PEO over a broad range of M_w. The study suggests the utility of reduced-order fractional modes as a tool for developing predictive relations which could conceivably be inputted into material design workflows.

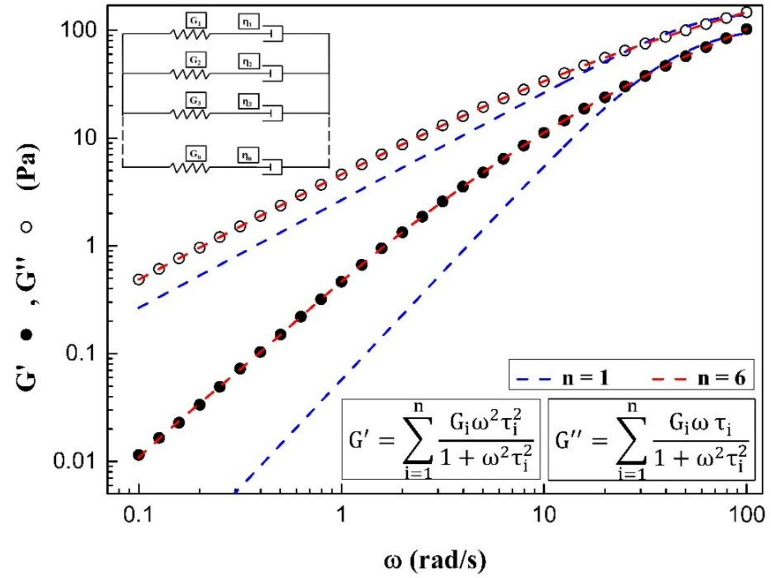

Figure 1: Oscillatory storage (G') and loss (G") modulus of a 300kDa PEO at 7.5wt% in water comparing the fit for 1 vs 6 maxwell modes.

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Modeling Local and Collective Dynamics in Polymer Grafted Nanoparticle Systems

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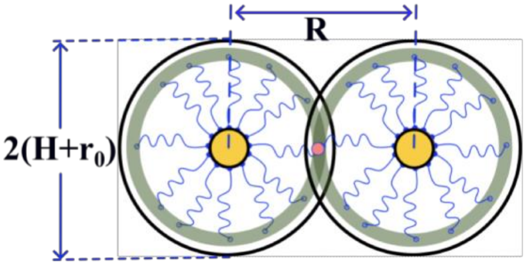
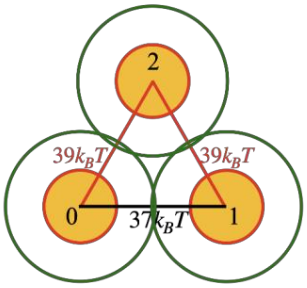
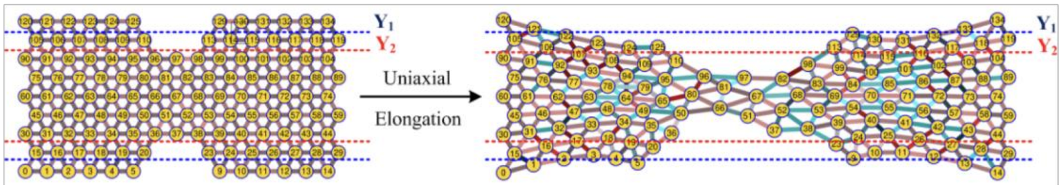
The assembly and properties of networks formed from polymer grafted nanoparticles (PGNs) can be tuned by a variety of parameters like density and length of the polymer grafts, shape and size of the particles on which polymers are grafted and the energy of the functional cross-links between interacting PGNs. To aid rational design of PGN composites we develop multicomponent models and multi-scale simulations using self-consistent field theory and stochastic approaches. Employing these models and simulation tools we examine rheological and mechanical properties of networks composed of PGNs with (a) varying number of grafts, (b) length of the grafted chain and (3) functional interactions. The results reveal that both the local linear and non-linear rheological response strongly depends on the grafting density and functional interactions. Further, we show that features like ductility, toughness and relaxation time depend strongly on the Deborah number.







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Single contaminated droplet microextraction in a yield-stress fluid

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The flow of a solute across a dispersed and a continuous phase has become an extensive research area owing to its numerous applications. It is known that the rate of mass transfer and chemical reactions are governed by the flow field around the bubbles present in the system. This mass transfer has immense value in the systems where liquid/liquid interaction takes place. In such systems, interfacial tension is dependent on the solute concentration [1]. Droplet systems are full of impurities or surface-active materials. These contaminants can reduce the internal circulation of the droplet system, and thus increase the drag, thereby reducing the overall heat and mass transfer rates [2]. The present work investigates the flow and mass transfer around a contaminated drop dispersed in a Bingham plastic fluid. Stagnant-cap model has been employed in this study in a Non-Newtonian fluid.

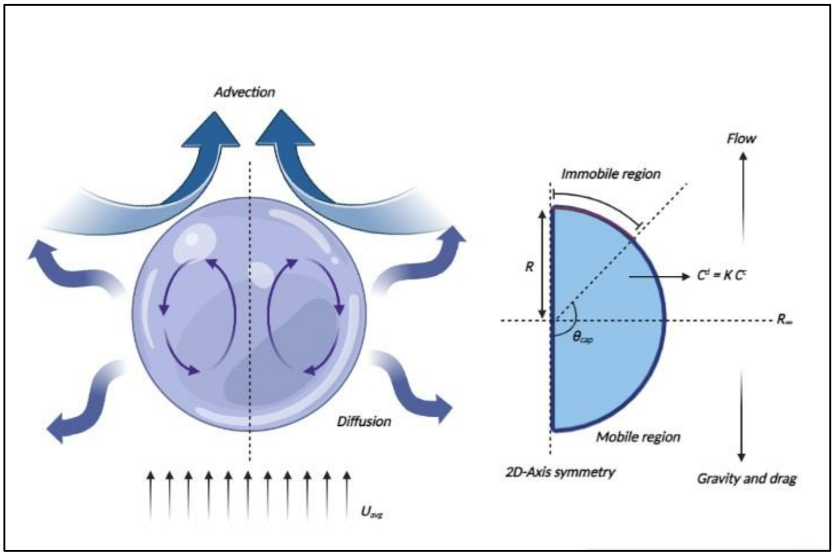

Figure 1: Schematic representation of a contaminated Newtonian drop falling in a Bingham fluid.

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Non-equilibrium dielectric relaxation of a nematic liquid crystal

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We study the dielectric dispersion of a nematic liquid crystal under steady shear. We find that the dielectric relaxation frequency strongly dependent on the shear rate. In particular, the relaxation frequency initially decreases and then increases beyond a particular shear rate. The shear induces a curvature strain which is zero for zero shear rate and is negligible for higher shear rates whereas it is maximum for some intermediate shear rates. This can give rise to flexoelectric polarization for intermediate shear rate range. Our experiments demonstrate a possible coupling of flexoelectric polarization to the dielectric polarization.

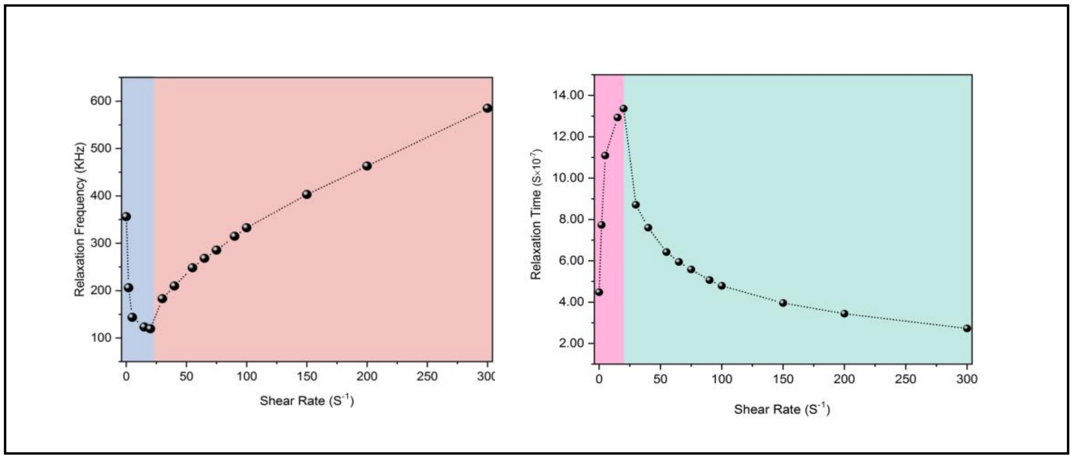

Figure 1: Schematics showing the dependence of dielectric relaxation frequency and dielectric relaxation time on the applied shear rate.

The relaxation time obtained from the Havriliak Negami function increases initially and then decreases whereas the relaxation frequency decreases initially and then increases beyond a particular value of shear rate. This observation indicate the emergence of flexoelectric polarization for the intermediate shear rates.

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Non-linear Rheology of Polymer Grafted Nanoparticle Solutions

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Polymer-grafted nanoparticles have gained significant attention due to their tunable properties and potential applications in various fields, including nanomedicine, separation membrane, and adhesives [1]. The collective structure of polymer-grafted nanoparticles (GNP) solution can be tuned by adjusting the grafting concentration, polymer length and nanoparticle loading. This enables control over parameters like stability, conductivity, gas permeability and rheology [2]. However, the composition-structure-property correlation is not fully understood. Here, we perform large-scale computer simulation and report a dispersion to aggregation transition of a GNP solution. We further establish a connection between the rheology of the materials and morphological transition. At a threshold value of GNP concentration there is a significant increase in the viscosity of the composite due to the aggregation of GNP in the matrix. This transition is further tuned by the grafting concentration of polymer chains in a nanoparticle surface as shown in Figure 1. High grafting enhances the miscibility and solubility of NPs in the solvent. It imparts mechanical strength to the material, making it stiffer and more resistant to deformation. The transition from dispersion to aggregation determines the point at which the material transits from a liquid-like behavior to a gel-like behavior. Overall, the dispersion to aggregation transitions leads to a non-monotonic change in the rheology of the material.

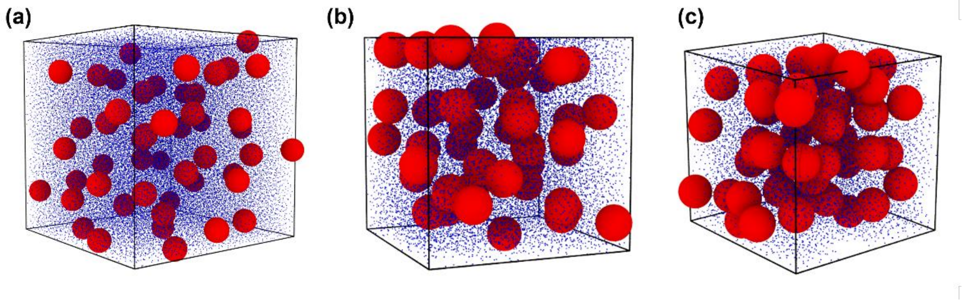

Figure 1: CGMD simulation of GNP solution. The MD snapshots for NP loading 0.07, 0.25 and 0.35 are shown in (a), (b) and (c), respectively, for a given grafting concentration red spheres are NPs and blue points are solvent particles.

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Effect of Geometric Disorder on Chaotic Viscoelastic Porous Media Flows

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Many practical applications, such as enhanced oil recovery or groundwater remediation, encounter the flow of viscoelastic fluids in porous media. Once the flow rate exceeds a critical value in such flows, an elastic instability with a fluctuating flow field is observed, which ultimately transits to a more chaotic and turbulence-like flow structure as the flow rate further increases. In this study [1], we present an extensive numerical investigation of the viscoelastic fluid flows in a model porous media consisting of a microchannel with many micropillars placed in it by considering both their initial staggered and aligned configurations. Within the present range of conditions encompassed in this study, we find that the geometric disorder always increases the chaotic fluctuations irrespective of the initial arrangement of micropillars. We propose that it is due to the formation of preferential paths or lanes and the formation of highly curved streamlines, which results in the local stretching of polymer molecules and, hence, significant origin in the local elastic stresses. We further show that this chaotic flow behaviour strongly depends on the competitive influence between the strain-hardening and shear-thinning behaviour of a viscoelastic fluid, which again strongly depends on the polymer extensibility parameter, polymer viscosity ratio, and geometric disorder parameter. In particular, we show that the strain-hardening behaviour of a viscoelastic fluid promotes these chaotic fluctuations, whereas the shear-thinning behaviour tends to suppress these. Therefore, it is not a general phenomenon that can always be seen in the flows of a viscoelastic fluid in porous media.

Keywords: viscoelastic, porous media, elastic instability, shear-thinning.

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Purely Elastic Center-mode Instability in Dean Flow

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Viscoelastic fluids are well known to undergo `purely elastic' linear instabilities in curvilinear geometries such as the Taylor-Couette or Dean flow configurations, driven by hoop stresses, even in the absence of fluid inertia. In a marked departure from this paradigm, recently Khalid *et al*. [1] predicted a linear `centermode' instability for plane Poiseuille flow in the limit of highly-elastic, ultra-dilute polymers solutions, with the solvent to solution viscosity ratio $\beta > 0.99$. The novel instability is driven by a critical-layer mechanism that does not rely on a base-state hoop stress.

The objective of the present effort is to demonstrate the existence of an analogous centermode instability in viscoelastic Dean flow, entailing pressure-driven flow in a curved channel. While it might be expected that the centermode (CM) instability would also be present in Dean flow in the narrow-gap limit (viz., gap width much small compared to the radius of curvature of the channel), the present work shows that the CM instability is present even for finite O(1) and larger values of the gap-width ratio. The instability is present in the limit of purely nonaxisymmetric disturbances only in the azimuthal (flow) direction, but continues to exist even when the disturbances vary in both azimuthal and axial directions.

This is in contrast to the hoop-stress mode (HSM), which is primarily axisymmetric, but continues to be present even for nonaxisymmetric disturbances. We show parameter regimes in the Wi-ε-β space where the CM and HSM are present. Our results show that, within the Oldroyd-B model, the HSM still remains the most critical mode in viscoelastic Dean flow for $0.01 < \varepsilon < 10$. We anticipate, however, that upon use of the more accurate FENE-P model, the critical Wi for CM would become comparable or lower than that of HSM, thus making the observation of the CM instability potentially feasible in viscoelastic Dean flows.

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Elastic center-mode instability in viscoelastic plane Couette-Poiseuille flow

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We analyze the linear stability of viscoelastic channel flows, with velocity profiles that are asymmetric about the channel centerline, belonging to the one-parameter Couette-Poiseuille family (CPF). These flows are driven by a combination of an imposed pressure gradient and (tangential) wall motion. A particular member of this family, corresponding to a zero net volumetric flux, may be experimentally realized in a shallow lid-driven cavity flow configuration, as well as in the narrow-gap limit of the Taylor-Couette geometry with an obstruction at a fixed azimuthal angle (a narrow gap Taylor-Dean flow). Recent work by Khalid *et al.* [1] has shown, using the Oldroyd-B model, that plane-Poiseuille flow with a symmetric velocity profile becomes unstable, even in the absence of inertia, to an elastic 'center mode' with phase speed close to the base state maximum. In contrast, viscoelastic plane-Couette flow is linearly stable.

The objective of this study is to determine parameter regimes where viscoelastic CPF, whose members interpolate between the two limiting flows above, is unstable in the inertialess limit. The dimensionless groups that govern stability are the Weissenberg number $W = \frac{\lambda U_{avg}}{L}$, the parameter α characterizing the relative importance of Couette ($\alpha = 0$) and Poiseuille flow ($\alpha = 1$) components, and the ratio of solvent-to-solution viscosities $\beta = \frac{\mu_s}{\mu}$. Here, λ is the polymer relaxation time, L the channel half-width and U_{avg} the average speed; $\beta \in [0,1]$, and $\alpha \in [0,\infty)$ with $\alpha \gg 1$ representing the limiting flow in a shallow lid-driven cavity. We show that similar to plane-Poiseuille flow, an elastic center-mode instability does indeed exist for the aforesaid family in the limit of ultra-dilute polymer solutions ($\beta > 0.99$); the instability relies on the existence of a base-state maximum, implying its absence for CPF members with $\alpha < 0.25$. This particular feature also points to the potential relevance of the center-mode to viscoelastic Taylor-Dean flows and other curvilinear shear flow configurations.

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Rheological Behavior of Colloidal Silica Gel

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Soft glassy materials are a class of thermodynamically out-of-equilibrium soft materials that exhibit microstructural evolution under quiescent conditions, a phenomenon known as physical aging. Such materials also demonstrate thixotropy and may possess yield stress. In this work, we study the thixotropic and yield stress behavior of such a system composed of aqueous dispersion of colloidal silica. We study how the physical aging behavior in the same gets affected as a function of time elapsed since their preparation. We also study how the behavior changes upon the addition of a small amount of Laponite RD in the same. In this study, we systematically analyze the evolution of viscoelastic moduli, yield stress, and relaxation time as a function of waiting time with the changing rest time and clay concentrations.

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Fractional calculus derived empirical predictive relations for the linear viscoelasticity of semi-dilute polymer solutions

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The oscillatory viscoelastic functions of polymer solutions often exhibit a power-law response, of the form $G'(\omega) \sim \omega^{\alpha}$ which are not well modeled using canonical generalized Maxwell modes. Recently, there has been a strong revival in applying fractional order constitutive modes for studying the response of a variety of complex fluids. Here, using poly(ethylene) oxide (PEO) in water as a model system and Bayesian statistics, we demonstrate that modeling their frequency-dependent complex moduli entails upwards of 20-Maxwell modes whereas, an equivalent good-fit is obtained using a single mode fractional equivalent. This greatly reduces the dimensionality of the model parameters from $\in R^{\sim 40}$ to $\in R^{\sim 4}$. Furthermore, we study the $c - M_w$ dependence of the fractional model parameters and discuss an empirical relation for predicting different linear viscoelastic functions of semi-dilute aqueous solutions of PEO over a broad range of M_w. The study suggests the utility of reduced-order fractional modes as a tool for developing predictive relations which could conceivably be inputted into material design workflows.

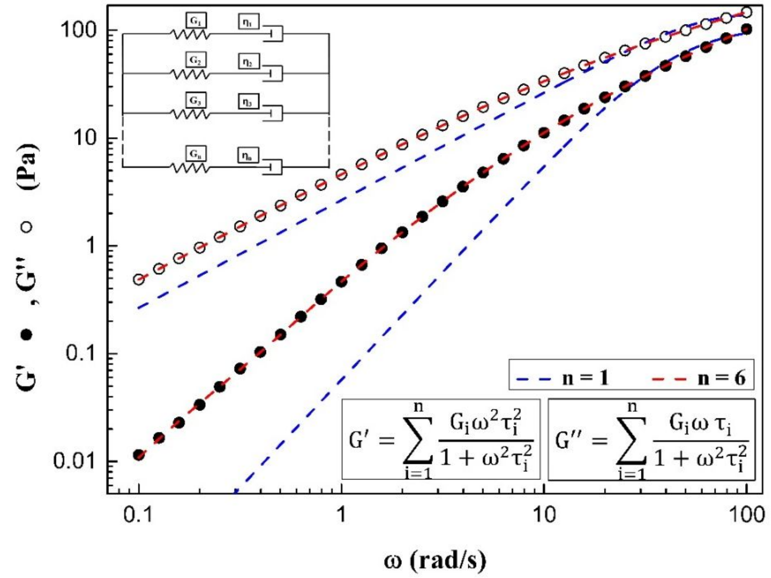

Figure 1: Oscillatory storage (G') and loss (G") modulus of a 300kDa PEO at 7.5wt% in water comparing the fit for 1 vs 6 maxwell modes.

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Indian Society of Rheology

Novel Periodic Shear Protocols: Understanding Rheology and RIT

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Suspensions are ubiquitous in our lives, examples being ink, paint, shampoo, yogurt, blood, etc. Yet it remains challenging to predict and control their flow properties accurately, due to the complex interplay between the external flow and the underlying microstructure, which further affects the suspension rheology. Even if the suspending fluid is Newtonian, suspensions can show complex rheological behaviors such as shear-thickening, shear-thinning, and yielding. The particle dynamics under cyclic shear show reversible-irreversible transition (RIT) at certain critical strain amplitude. These suspensions undergoing RIT also show certain rheological signatures like minimum viscosity at the critical strain amplitude, hinting at possible linking between the dynamics and rheology via microstructure.

In this work we propose novel shear protocols (refer to underlying figure): Rotary Shear (RS) and Reversible Rotary Shear (RRS) to investigate the link between the rheology and the dynamics and compare these novel protocols' behavior to the widely investigated Oscillatory Shear (OS) protocol. Specifically, we show that the suspension rheology is robust: there is a volume fraction-dependent critical strain amplitude at which the relative complex viscosity is minimum. However, the suspension dynamics are qualitatively different. While suspensions under RRS undergo RIT at a critical strain amplitude like OS, the same suspension remains inherently diffusive in RS. Finally, we discuss how periodically driven suspensions' rheological responses and dynamics are linked to the microstructure evolution.

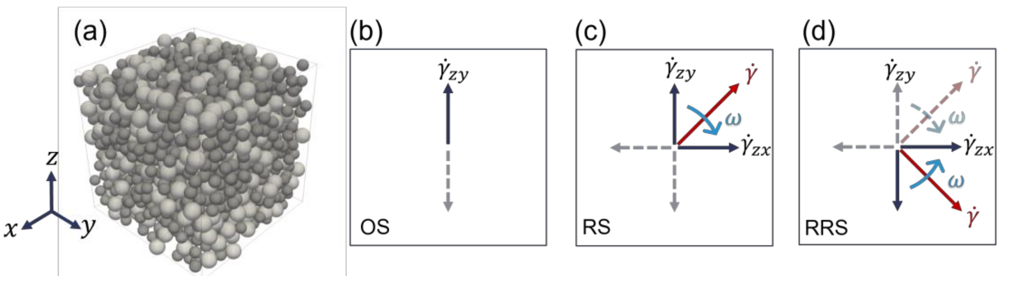

Figure 1: Schematic diagram of (a) particulate suspension, (b) OS, (c) RS, and (d) RRS.

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Flow around a local probe driven in wormlike micelles: origin of flow instabilities

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Fluctuations of bulk stress in turbulent flow of wormlike micelles are ubiquitous in Taylor-Couette flows. It has been observed that for 2wt% CTAT (cetyltrimethylammonium tosylate) and 100 mM NaCl based wormlike micellar solution, the steady-state stress fluctuations arises due to continuous breakage and reorganization of large scale structures formed during shear. However, understanding fluctuations from a local perspective is still not understood and characterized. Here, we study the onset of fluctuations and their microscopic origin by driving a local probe in the viscoelastic micellar solution. Interestingly, the breakage of shear induced structures are well correlated to the observed fluctuations in a one to one manner. However, the magnitude of such fluctuations are related to the length scale of shear induced structures. The time scales of breakage during unstable flows are comparable to the equilibrium breaking time which suggest an intriguing connection between them.

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Unveiling the enhanced magnetorheo-transport dynamics in magnetic ionic liquid

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Magnetic Ionic Liquids (MILs) belong to the classic and dynamic category of ionic liquids, exhibiting magnetism due to their inherent magnetic cations.[1] The ongoing research into their manufacturing and diverse applications, including drug delivery is fueling a growing interest in MILs for both the current and upcoming periods.[2] Unlike prior research improving magnetism in non-magnetic systems, our study innovates by enhancing magnetic properties in inherently magnetic systems. Here, our work aims to enhance the rheological flow behavior of MIL by incorporating nanoparticles. We examine how incorporation of nanoparticles and magnetic field intensity impacts the current magnetorheological system. A pristine MIL displays newtonian behavior. However, the introduction of nanoparticles (NPs) shifts this behavior to non-Newtonian in the absence of a magnetic field and in the presence of a magnetic field, viscosity increases, as illustrated in Figure 1. Further, to gain more insights into the magnetic behaviour of these system, we also assessed their susceptibility and saturation magnetization using vibrating-sample magnetometer (VSM) system. This approach provides insights into the enhanced transport properties of MIL through the NP addition, therefore, providing crucial information about their magnetic characteristics, making them potential candidate for emerging magnet-based technologies.

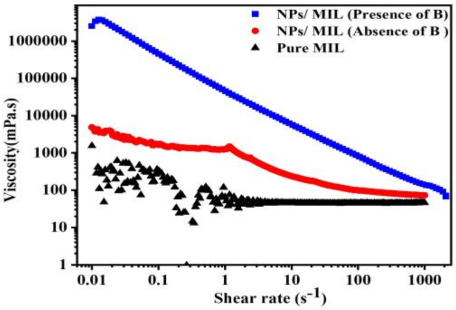

Figure 1: Viscosity versus shear rate measurement for pure MIL system, MIL with the nanoparticles in the absence and presence of magnetic field (B).

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First normal stress differences in model TEVP fluids

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Thixotropic-Elasto-Viscoplastic (TEVP) fluids exhibit various phenomenon such as shear thinning and yield stress in steady shear, viscoelasticity and thixotropy in transient shear tests. A model TEVP system developed by Dullaert and Mewis [1] has been extensively studied in various rheological protocols and different mathematical models. This model system in various steady and transient shear tests exhibits shear stresses with limited measurements of first normal stress differences. Due to this, the time scales associated with thixotropy and normal stress differences are not well understood and whether both these phenomena co-exist at the same time is not clear. Recently we developed a filled polymer melt as a model TEVP fluid that was reported to have improved viscoelasticity at lower times and longer structural breakdown scales in transient shear tests [2]. This filled melt also exhibits positive first normal stress differences at higher shear rates under steady shear. The material response of both shear stresses and first normal stress differences is quantified using two different three-dimensional constitutive equations from literature [3,4]. While both the models are observed to be quantifying the shear stress response well, significant deviations are observed in first normal stress differences that requires improvement in the existing models.

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An organogel programmed to spontaneously degrade: How a breakthrough in rheology can enhance oil production

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Gels are used in many applications in the oilfield, in medicine, and in consumer products. For example, during oil drilling, organogels are pumped underground into fractures within oil-bearing rock. The gel must then act as a solid plug to block the flow of liquid (oil or water). However, after a period of time (days to weeks), the solid gel must degrade (i.e., transform to a thin sol) to enable oil to be extracted. Such degradable gels are also sought after for many other applications. To degrade gels at a specific time, many 'degrading agents' as well as external stimuli (e.g., heat or light) have been examined. Here, we introduce a new concept that avoids both external agents and stimuli: we demonstrate *self-degrading organogels* that are (a) extremely strong and robust at time $t = 0$ and (b) degrade spontaneously into a sol after a set time $t = t_{deg}$ that can be minutes, hours, or days. This unprecedented combination of properties is achieved by simply combining two readily available molecules — the organogelator, (1,3:2,4)-dibenzylidene sorbitol (DBS) and an acid (e.g., hydrochloric acid, HCl) — in an organic solvent. DBS self-assembles into nanoscale fibrils, which connect to form a 3-D network, thereby gelling the solvent. The DBS concentration sets the gel strength, and just 2% of DBS is enough to make a robust gel (elastic modulus $G' > 10$ kPa) — such a gel can be picked up and handled as a free-standing solid. At the same time, the acid concentration sets the kinetics of gel degradation and thereby the value of t_{deg} at a given temperature. For example, a 2% DBS gel in ethylene glycol containing 10% of 0.5 M HCl degrades after 7 days at 25°C and after 2 h at 70°C. We use a combination of NMR and mass spectrometry to delineate the chemical mechanism for degradation. The acid is shown to induce a slow hydrolysis of the acetal groups, thereby converting DBS into a form that cannot self-assemble into fibrils. Self-degrading DBS gels with a pre-programmed 'degradation clock' can be made with both polar and non-polar organic solvents and thus have wide-ranging applicability. The concept could be a game-changer for oil recovery as it promises to make the process more efficient and sustainable (due to reduced consumption of drilling fluids).

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Insights on Slip-layer Dynamics Using Electrorheology

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The phenomenon of wall slip is ubiquitous in industrial and natural flows of various soft materials (emulsions, foams etc.), occurring over a broad range of length scale: from microfluidics flows to hydraulic transport of complex dispersions. Such slip occurs near the wall due to formation of very thin layer (~ few nm to µm) of low viscosity, termed as *slip-layer*, having velocity gradient within it. Slip layer is very crucial in correct experimental estimation of rheological properties and understanding various flow regimes. Therefore, deep understanding of slip behaviour along with its characterization is of great significance from industrial as well as academic point of view. In this work, we have studied how extent of jamming effects on wall slip characteristics using Electrorheological Fluids, which is a model anisotropic soft-jammed material. The extent of jamming in such fluids can be controlled by external electric field at a fixed concentration. We have experimentally generated pure elongation flow in order to estimate slip-layer thickness as a function of electric field intensity. The current investigation provides new insights on wall slip phenomenon bulk anisotropic soft-jammed systems, in general, especially to understand the role of jamming towards slip dynamics.

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Numerical simulations for electro-osmotic flow of PTT fluids in diverging microchannel.

Technical Presentation

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Abstract

In recent years, the development of microfluidic devices has gained significant attention, particularly in the areas of environmental considerations, pollution control for water contamination measurement, and microbial activity detection. These devices also find applications in diverse fields such as reaction engineering, healthcare, and separation processes. Consequently, there has been a growing interest in researching the design, flow kinematics, and control of microfluidic devices. One prominent aspect that has received substantial research focus is the use of electroosmotic forcing, which offers great adaptability and applicability in microscale flow. Over the past three decades, numerous studies have accumulated, providing a comprehensive overview of the advancements in this field. These studies have explored various aspects of electroosmotic forcing in microfluidics devices, contributing to the understanding and utilization of this phenomenon in a wide range of applications [1].

In this study, we have conducted a numerical investigation of electroosmotic coupled pressure-driven flow in a diverging microchannel using simplified Phan Thien Tanner (PTT) fluids. To linearize the electric potential distribution in the electric double layer, we employed the Debye-Hückel approximation, with a fixed Debye length ($\kappa H = 20$). The coupling of pressure and electroosmotic forces was considered, and a forcing ratio (Γ) was varied within the range of -4 to 4, representing the ratio of pressure to the electrokinetic gradient in the flow direction. The rheology of the viscoelastic fluid was influenced by both the characteristic Deborah number and the PTT parameter, with values ranging from $0.1 \leq (\sqrt{\varepsilon} De) \leq 5$. Moreover, we analysed the impact of the divergent angle (α) withing the range of 5^{o} to 15^{o} degrees to understand how channel geometry affects the resulting flow kinematics. To present and discuss the outcomes, we visualized variation in the flow field using velocity vectors, surfaces, and velocity profiles at the outlet of the microchannel. The study provides insights into the flow behaviour and sheds light on the role of various parameters on the flow characteristics in the investigated microfluidic system.

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Rheological behaviour of Aqueous alumina suspension for Direct Ink writing process

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Direct ink writing is the process in which a suspension with high ceramic loading (> 45 Vol %) is extruded through a nozzle in filament shape for near net shape fabrication of ceramic parts [1]. In present work the rheological properties of aqueous Alumina suspension (up to 58 Vol%) has been presented. The suspension has been prepared using α- Alumina, water soluble PVP as stearic stabilizer and NHPA as electrolytic stabilizer. The flow behaviour of the PVP and NHPA containing suspensions showed yield-pseudoplastic characteristics which has been closely agreed with the Herschel–Bulkley fluid model. The addition of PVP, NHPA and PEG significantly changed the rheology of the suspension system, increasing the shear yield stress and changing flow behaviour. The flow behaviour of suspension directly affects the 3D printing of ink [2]. The shape retention of ink filament defines the structural stability of the part to be printed. Figure 1 shows direct ink writing with a stable suspension. Rheological behaviour of the ink plays the most important role in Direct ink witing process.

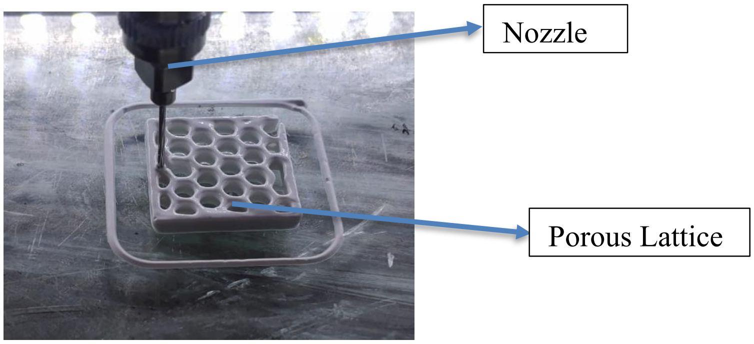

Figure 1: Direct Ink writing of Alumina suspension

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Dynamics of spherical particles in the presence of shear and oscillating magnetic field

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The dynamics of a spherical particle in the presence of shear and an oscillating magnetic field in the shear plane, is defined in terms of the dimensionless numbers ω^*, which is the ratio of the magnetic field frequency and the shear rate, and Σ, which is the ratio of the magnetic and hydrodynamic torques. As the magnetic field strength is increased, Σ increases and the behavior of the particle evolves from close to Jeffery orbit like to synchronized rotations in the shear plane. When $\omega^* < 1/2$, this phase locking displays Arnol'd tongue at $\omega^* = \frac{1}{2\, n_0}$, where n_0 is an odd integer, and then discontinuous change in the rotation number as shown in figure 1. The hydrodynamic torque exerted by the particle on the fluid changes as the behavior of rotation of the particle changes.

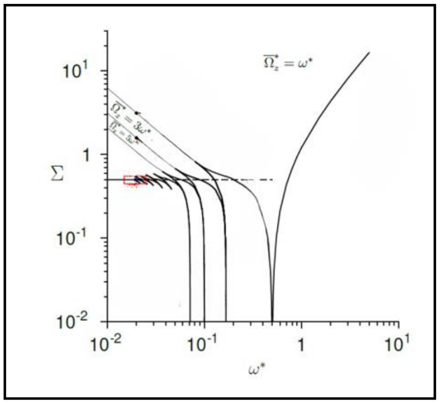

Figure 1: The boundary between rotations in the plane of the flow (regions topologically connected to $\Sigma \gg 1$) and not in the plane of flow (regions topologically connected to $\Sigma \ll 1$) in the $\omega* - \Sigma$ parameter space. $\overline{\Omega^*}_z$ is the particle angular velocity.

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Effects of local incompressibility on the rheology of composite biopolymer networks

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Fibrous networks such as collagen are common in biological systems. Recent theoretical and experimental efforts have shed light on the mechanics of single component networks. Most real biopolymer networks, however, are composites made of elements with different rigidity. For instance, the extracellular matrix in mammalian tissues consists of stiff collagen fibers in a background matrix of flexible polymers such as hyaluronic acid (HA). The interplay between different biopolymer components in such composite networks remain unclear. In this work, we use 2D coarse-grained models to study the nonlinear strain-stiffening behavior of composites. We introduce a local volume constraint to model the incompressibility of HA. We also perform rheology experiments on composites of collagen with HA. We demonstrate both theoretically and experimentally that the linear shear modulus of composite networks can be increased by approximately an order of magnitude above the corresponding moduli of the pure components. Our model shows that this synergistic effect can be understood in terms of the local incompressibility of HA, which acts to suppress density fluctuations of the collagen matrix with which it is entangled.

Physical Aging Behavior of Aqueous Solution of Pluronic F127

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Abstract

Pluronic polyols, commonly known as poloxamers, consist of central poly(propylene oxide) blocks flanked by poly(ethylene oxide) blocks. Amongst these tri block co polymers, F127 exhibits an interesting thermo responsive phase behavior wherein it undergoes sol-gel and gel-glass transition depending on its concentration in the aqueous solution and the temperature. Pluronic F127, when subjected to temperature variations, including a sudden increase from sol state to a specific temperature point in the glass phase, or quenched from a high temperature viscoelastic liquid region to the same point, its rheological properties evolve as function of time under isothermal conditions. Furthermore, after cessation of shear flow (mechanical rejuvenation), F127 shows physical ageing. In this work, we evaluate two rheological properties – dynamic moduli and creep compliance at different waiting times post two types of thermal rejuvenation as well as mechanical rejuvenation. We also perform time waiting time superposition of the compliance data and observe that the system displays a similar sub-ageing behaviour in all the cases.

Use of multi-wave rheological technique to characterise bitumen at low temperatures

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The rheological response of bitumen depends on temperature and during the pavement service period, especially at low temperatures between 0 and 30 ℃, it exhibits a viscoelastic solid to elastic solid response. Such responses are also strongly influenced by the frequency of loading and it is hypothesised that for a given range of frequencies, the degree of dependence on frequency decreases with decreasing temperature as the material response transits from viscoelastic solid to elastic solid. An ideal way of capturing this response is by performing isothermal frequency sweep experiments at various temperatures. However, this is time consuming and an alternate way to explore this response would be to use a multi-wave technique.

A multi-wave technique is one in which loading in the form of a series of sinusoidal waveforms is applied to the sample simultaneously rather than a single waveform sequentially as in a frequency sweep experiment. This technique has been widely explored in the field of polymer science and finds its usefulness in identifying the gelation point and also acts as a substitute for frequency sweep tests on materials whose structure evolves with time. This technique helps in probing the bitumen at different frequencies simultaneously and to make effective use of this technique, it is desirable to accommodate as many waveforms as possible in the multi-wave while ensuring that the material response is linear.

Taking this into consideration, this study focuses on establishing a test protocol for the multi-wave technique by optimising the parameters required to generate the multi-wave (frequency, strain amplitude, number of waveforms and phase shift). With the optimised parameters, the multi-wave is applied to bitumen in the temperature range of 0 to 30 ℃ and the frequency dependent parameters such as storage modulus, loss modulus and phase angle obtained by post-processing the multi-wave data are observed for their dependence on frequency with temperature. The results are also compared with that of conventional frequency sweep experiments.

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Influence of Frequency and Temperature on Warping Stress in Bituminous Mixture

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Bituminous mixtures used in highways and runways consist of aggregates of different sizes bound together by bitumen and fillers (material passing 0.075 mm). These mixtures exhibit viscoelastic response under service conditions. Bituminous mixtures are characterised by different loading conditions, such as tension-compression, compression and flexure. The viscoelastic response of the bituminous mixture is due to the presence of bitumen, and subjecting the mixture to torsion gives a better characterisation of the viscoelastic material in the mixture. ASTM D7552 (2022) [1] gives a test protocol to characterise bituminous mixtures in torsion using a dynamic shear rheometer (DSR). The standard prescribes using a prismoidal (rectangular cross-section) specimen geometry for testing. These prismoidal specimens have a non-axisymmetric cross-section, leading to the development of warping stresses in the DSR where the specimen ends are restrained. The effect of warping stress is not constant across frequencies and temperatures for a viscoelastic material and can vary depending on the material's properties. Several other researchers have used cylindrical (circular cross-section) specimen geometry for testing bituminous mixtures in torsion. The cylindrical specimen has an axisymmetric cross-section and thus does not warp nor produce warping stress when subjected to torsion in a DSR. A comparison between the linear viscoelastic properties of the two specimen geometries for a bituminous mixture has not been conducted.

In this investigation, two bituminous mixtures of cylindrical and prismoidal specimen geometries having the same material constitution are tested using a DSR. A frequency sweep experiment is carried out for frequencies ranging from 0.01 Hz to 20 Hz, and the test temperatures are 10, 20 and 30 °C. Torque and deflection angle are the two raw values obtained from the DSR. These raw values are converted to absolute shear modulus using equations given by Mezger (2020) [2]. These equations are based on the theory of pure torsion and do not consider warping stresses. Therefore, the linear viscoelastic properties of a prismoidal bituminous mixture obtained from a DSR have two components: a material-based component and a geometry-based component. The absolute shear modulus of the two specimen geometries is observed to differ, with the prismoidal specimen having a higher modulus value across all frequencies and temperatures. Correction factors based on linearised elastic theories are available for delineating the geometry-based component from the properties obtained from the DSR for a prismoidal specimen. There are several challenges associated with the application of these correction factors for a viscoelastic material like bituminous mixtures.

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Indian Society of Rheology

Apparent viscosity and shear rate dependency characterization of reclaimed asphalt pavement (RAP) binders

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Abstract

Considering the dearth of natural resources such as aggregate and bitumen, the current impetus of the world-over is to use recycled bituminous mixtures. The bitumen available in the aged highway has considerably different rheological properties when compared to virgin bitumen. The industry practice is to add rejuvenating agents (RA) to the aged bitumen so that it can be amenable for use in subsequent construction. Most of the existing RA play the role of a solvent, and very rarely the underlying rheological properties are 'rejuvenated'. In addition, it is also required to determine the rheological properties of a mixture of aged bitumen, RA and virgin bitumen. This investigation will focus on determining the rheological properties of such a complex mixture by measuring the flow curve and use this to quantify the extent of rejuvenation at the macroscopic scale.

The materials used in the study are a binder extracted from an existing highway, a commercial RA and an unaged polymer-modified bitumen. All the materials are subjected to a shear rate sweep experiment using parallel plate geometry. The experiments are conducted at three critical temperatures of 50, 60, and 70 °C. The flow curves of the aged bitumen, virgin bitumen, and RA blends indicate significant variations in the extent of shear thickening followed by shear thinning. The rate of shear thinning and thickening are observed to be temperature dependent. It is seen that the addition of a rejuvenator influences the shear-thickening and shear-thinning characteristics of the blend.

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Indian Society of Rheology

Investigation of the Various Relaxation Modes for a Class of Bituminous Mixtures

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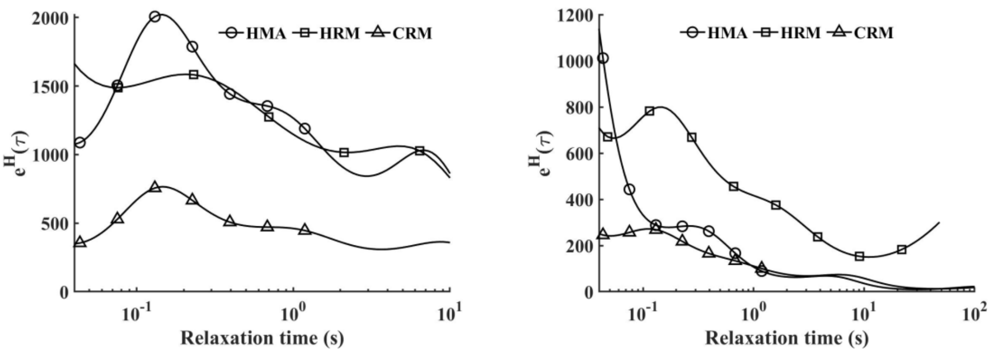
A typical highway/runway bituminous pavement consists of two layers of bituminous material on the surface. Over its service life, the bituminous layers deteriorate, and they need to be rehabilitated. Such rehabilitation can use existing bituminous material, or it can consist of providing an additional layer with virgin materials. Many technologies exist related to the use of existing bituminous material. One such technique uses cold recycling technique, while the other technique uses hot recycling. It is expected that such materials made with such disparate technologies are expected to have identical load-carrying capacity quantified in terms of linear viscoelastic parameters such as dynamic modulus and an associated master curve. Since each of these methods, virgin material (HMA) and recycled materials (hot (HRM) and cold recycled mixture (CRM)), are different, it is expected that the mechanical response is also different. However, since the measurements are conducted in the linear viscoelastic regime, a refined analysis of the underlying response is needed to quantify these differences precisely. This study focuses on the use of the relaxation spectrum towards this purpose.

The experimental phase involves conducting dynamic mechanical analysis through repeated haversine compression load tests over various temperatures and frequencies to capture dynamic modulus and phase angle. The modelling phase involves the construction of isothermal relaxation spectra using the dynamic modulus data set corresponding to each temperature. The isothermal relaxation spectrum is further deconvoluted to discern distinct relaxation modes and their associated characteristics. Such an exercise of characterising and understanding the different relaxation modes will enable to gain deeper insights into the viscoelastic response of the different classes of bituminous mixtures under consideration. Figure 1 compares the relaxation spectrum of the three mixtures under consideration at two different temperatures. Notably, at 25°C, HMA and HRM exhibit identical relaxation characteristics, while at 45°C, HMA's response matches that of CRM.



(a) 25°C (b) 45°C

Figure 1. Comparison of the relaxation spectrum

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On the Arrhenius response of aged bituminous binders

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The bituminous binder used for pavement construction undergoes aging due to the high temperatures prevalent during the mixing and compaction process, generally referred to as short-term aging. Subsequently, prolonged exposure to environmental effects during the service period will result in aging, which is called long-term aging. Due to such aging, the chemical composition and, thus, the rheological properties of the aged bitumen will be distinctly different from that of the unaged bitumen. Also, the rheological response during the service life of the pavement is greatly influenced by the temperature sensitivity of bitumen.

In the study, the focus is on evaluating the change in the temperature dependency of bitumen with aging. Owing to the evolution of bitumen composition with aging, the temperature sensitivity of the bituminous binder needs to be captured at different aging conditions. Limited research is available on the variation in temperature sensitivity of bitumen with aging. While there are several measures to quantify temperature sensitivity, those attempts are largely based on parameters measured at a few temperatures, such as apparent viscosity and penetration. Studies have found that the Arrhenius relationship can reasonably describe the temperature sensitivity of bitumen. The Arrhenius relationship can also be useful to demarcate the phase transition in the material at different stages of aging.

The current investigation focuses on utilising the Arrhenius relation to ascertain the temperature sensitivity of bitumen at different extents of aging. An unaged unmodified bitumen of Viscosity Grade 30 (VG30) is chosen as the base binder for the investigation. Different extents of aging were simulated using short-term and long-term aging procedures available for binder aging in the laboratory. Bituminous binders of different ages were then subjected to frequency sweep test in the linear viscoelastic regime at 0.05% strain amplitude over temperatures ranging from 25 to 75°C using Dynamic Shear Rheometer. The Arrhenius relation was then fit to the absolute shear modulus, and the model parameters were used to quantify the influence of aging on the temperature dependency of bitumen.

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SM-06

Extending self-assembly beyond water: Wormlike micelles and vesicles in polar solvents at sub-zero temperatures

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Self-assembly of surfactants and lipids in water results in different structures, including long cylindrical chains called wormlike micelles (WLMs) as well as nanoscale containers called vesicles. However, in solvents of polarity lower than water (such as glycerol, formamide, or ethylene glycol), self-assembly of WLMs and vesicles has not been reported previously.

Recently, we have demonstrated, for the first time, that both WLMs and vesicles can indeed be formed in polar solvents [1-3]. Our work thereby extends self-assembly to new systems and, in turn, to extreme conditions such as sub-zero temperatures. Applications for these systems could arise in cosmetics, pharmaceutics, antifreeze agents, and lubricants.

To form WLMs in polar solvents like glycerol, a cationic surfactant with a very long (erucyl, C22) tail and an aromatic salt such as sodium salicylate are both needed [1]. These WLMs also have unusual rheology: they exhibit a double-crossover of their elastic (G') and viscous (G'') moduli within the typical range of frequencies [2].

To form vesicles in polar solvents, we use the simple phospholipid, lecithin [3]. Lecithin dissolves readily in these solvents and gives rise to viscous fluids at low concentrations (~ 2%). At higher concentrations (> 10%), lecithin forms clear gels that are strongly birefringent at rest. We show that the latter are 'vesicle gels', where multilamellar vesicles (onions), with sizes between 50 to 600 nm, are close-packed.

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Unveiling Guest Molecule Induced Alterations in Model Membranes

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Model membranes serve as simplified yet representative systems that mimic the structural and functional attributes of biological membranes, providing a controlled environment to unravel the intricate mechanisms underlying molecular interactions. We have studied two phenomena where the drug induces alteration in the cationic bilayer and the thermodynamics of pore formation and crossing behavior of DMSO in the bilayer.

To determine the potency of a drug carrier for the protected encapsulation of aspirin at different temperatures, united-atom molecular dynamics simulations of a model bilayer, dioctadecyldimethylammonium bromide (DODAB), are performed in the absence and presence of aspirin. The bilayers are in the interdigitated two-dimensional square phases at 298 and 310 K, which become rugged in the presence of aspirin. Aspirin is preferentially located near the headgroup and creates space, increasing the interdigitation and order parameters. Despite the structural arrest of the lipid center of mass, they reach the diffusive phase faster and exhibit higher lateral diffusion constants in the presence of aspirin. Energetics show aspirin insertion is most favorable at physiological temperature. [1] Thus, the ordered, more stable, and faster DODAB bilayer can be a potential drug carrier for the protected encapsulation of aspirin. Our findings comply with the DSC and QENS studies. [2]

At temperatures above the phase transition temperature of DMPC, detailed all-atom molecular dynamics simulations of 1,2-dimyristoylphosphatidylcholine (DMPC) bilayers are performed at different DMSO concentrations. Our findings show that DMSO partly dehydrates the interface and inserts itself between lipid heads without completely dehydrating it. Even at the greatest DMSO concentration examined, this results in a larger area per head group, a higher disorder, and enhanced fluidity without disintegration. The increased disorder promotes local fluctuations at the interface, which form dynamic and temporary pores. When water aids in the emergence of DMSO pores, the energy needed for pore formation reduces. The presence of interface water reduces the free energy of pore formation. The presence of interface water causes the formation of a two-dimensional percolated water-DMSO structure at the interface, which would not have occurred otherwise. [3]

By unveiling the nuanced alterations induced by guest molecules, a fundamental understanding of membrane behavior will pave the way for innovative applications in drug delivery, biomaterial design, and other biotechnological advancements.

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Protein machines and lipid assemblies: interdependence in membrane fusion

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Membrane fusion is an essential process for the survival of eukaryotes and the entry of enveloped viruses into host cells. A proper understanding of the mechanism of membrane fusion would provide us with a handle to manipulate several biological pathways and design efficient vaccines against emerging and re-emerging viral infections. Though fusion proteins take the central stage in catalyzing the process, the role of lipid composition is also of paramount importance. Lipid composition modulates membrane organization and dynamics and impacts the lipid-protein (peptide) interaction. Moreover, the intrinsic curvature of lipids has a substantial impact on the formation of stalk and hemifusion diaphragm. It has been shown that the insertion of fusion peptides into the host membrane and the perturbation in the membrane generated thereby is crucial for membrane fusion. Significant efforts have been made in the last couple of decades to understand the lipid-dependence of structure and function of the fusion peptide in membranes to understand the role of lipid compositions in membrane fusion. In addition, the lipid compositions further modify the membrane physical properties and alter the mechanism and extent of membrane fusion. Therefore, lipid compositions modulate membrane fusion by changing membrane material properties and altering the structure of the fusion peptide.

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Indian Society of Rheology

Assembling of DNA macromolecules at air-water interface

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Deoxyribonucleic acid (DNA) is a negatively charged bio-macromolecule that helps in the transmission of genetic information for the growth and functioning of a living organism. Therefore, it is considered as a potential tool in gene therapeutics. Packing or condensing of this macromolecule is difficult because of the intra and inter molecular repulsive electrostatic and entropic interactions. Even though there are reports of condensing the molecule using inorganic salts in bulk aqueous medium, the assembly at the air-water interface is rarely reported. Here, we report the assembly of the DNA molecule at the interface induced by an imidazolium based ionic liquid (IL) 1,3 didecyl-2-methylimidazolium chloride. The surface pressure-area isotherm ensures the presence of the molecule at the interface with a high mean molecular area. Interfacial rheology quantifies the elastic nature of the molecular film. The storage and loss modulus of the film is found to strongly depend on the in-plane pressure. Advanced in-situ synchrotron X-ray scattering study relates these physical properties of the film with its structure. The electron density profile of the film across the interface manifests the compact nature of the film in presence of the IL (Figure 1). This work suggests an easy way of immobilizing the DNA macromolecule at the air-water interface which can be used for future technological applications.

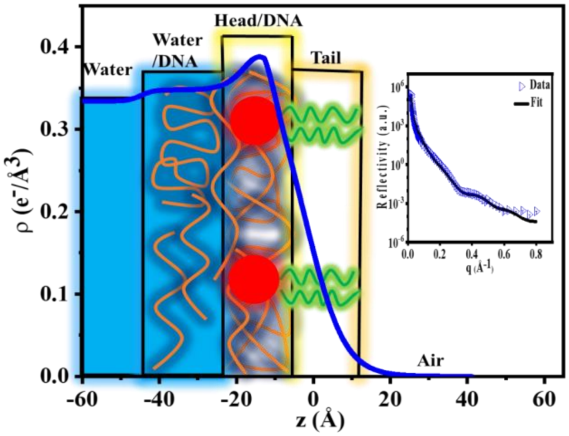

Figure 1: Schematic of assembly of DNA at air-water interface induced by ionic liquid. The continuous blue line is the electron density profile extracted by fitting an X-ray reflectivity profile shown in the inset.

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Interactions of cellular metabolites with membranes

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The interactions of cellular metabolites with membranes of complex composition has not been well studied. In general, small molecule binding is well characterized in terms of drug membrane permeability or binding energetics. The emerging concepts in metabolite-membrane interactions suggest that for several metabolites binding to membranes constitutes a key step for their final biological function [1], either by modulating membrane properties or by interacting with a partner within the membrane. We will present our current understanding on the interactions of a few plant metabolites, neurotransmitters and hormones. We have tested computational frameworks to analyze these interactions with both atomistic and coarse-grain resolutions. We analyze the interactions of these molecules with membranes of varying compositions and analyse the differences in binding modes and interactions. We observe that several of these metabolites are polar in nature and remain bound at the head-group region of the membrane. We have further identified differences in how they modulate membrane properties including lipid component demixing, fluidity and lipid packing. A few rare events such as bilayer translocations are identified and we delineate the pathways for such events. Our work is an important step in understanding the complex nature of the metabolite-membrane interactions.

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Unraveling Interactions between Ionic Liquid and DPPC Membrane

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A comprehensive investigation of the interaction between ionic liquids (ILs) and model cell membranes is essential for gaining detailed insights into IL toxicity and its potential applications in the pharmaceutical industry. In this work, we present a molecular dynamic simulation study to investigate the effect 1-decyl-3-methylimidazolium bromide ($DMIM^+$ $[Br^-]$) ILs on the dipalmitoylphosphatidylcholine (DPPC) membrane. The snapshots of DPPC+IL simulation at 303 K and 330 K are shown in Fig. 1(a) & (b), respectively. Below 314 K, DPPC molecules form the gel phase, with an area per lipid (APL) of 46 $Å^2$, as shown in Fig. 1(c). This APL value in the gel phase is consistent with the results from other simulations studies [1, 2]. In this phase, the alkyl chains are ordered, as indicated by an order parameter >0.35 (Fig. 1(d)) and a lower *gauche*/*trans* ratio (inset of Fig. 1(d)). The presence of ILs during this phase has minimal impact on these factors, including the APL, order parameter, *gauche*/*trans* ratio. This suggests that the insertion of $DMIM^+$ molecules into the bilayer is limited in the gel phase, with the majority of them prefer self-aggregation into micelle-like structures (Fig. 1(a)) [3]. The main phase transition of DPPC bilayer is captured well in our simulations at ~ 314 K which is found to be consistent with differential scanning calorimetry (DSC) experiment (Fig. 1(c)). In the fluid phase, the APL of the pure DPPC is increases to 67 $Å^2$, the alkyl chains become disordered, and *gauche*/*tans* ratio increases. Interestingly, the presence of ILs in the bilayer leads to an early onset of phase transition at a temperature of 310 K. Following this phase transition, ILs cease to aggregate, enabling a greater proportion of IL molecules to readily insert into the bilayer (Fig. 1(b)). The presence of ILs induces disorder in the bilayer and increases APL at higher temperatures. It is notable that incorporation of IL substantially enhances the van der Waals and electrostatic interactions of the lipid bilayer, remaining a potential underlying cause of early onset of main transition. Our study provides microscopic insights on the destabilizing effects of IL on the cell membrane.

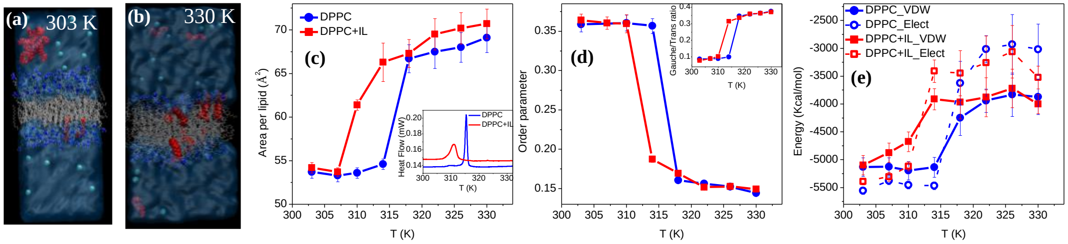

Figure 1. Snapshots of the DPPC+IL simulation at (a) 303 K and (b) 330 K. (c) APL and DSC data (inset). (d) Order parameter and *gauche*/*trans* ratio (inset), of the alkyl chain. (e) van der Waals (VDW) (solid lines) and electrostatic (Elect) (dashed lines) interactions.

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SM-P1

Self-assembly of graphene-based nano-materials in and around a lipid film

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The miracle material graphene and its subsidiaries namely, graphene oxide (GO) and reduced graphene oxide (rGO) have undergone extensive investigations due to their bactericidal properties as they disrupt a cellular membrane [1]. In the present study, Langmuir monolayers of zwitterionic, positively charged and negatively charged phospholipid molecules are subjected to structural commotions induced by graphene-based materials. These monolayers mimic one of the leaflets of a bilayer which is the structural matrix of a cellular membrane [2]. A Langmuir trough setup has been used where phospholipid monolayers are characterized by surface pressure-area and surface potential-area isotherms. The studies suggest specific attachment of GO to a positively charged phospholipid monolayer, while for rGO, major changes are observed for a zwitterionic monolayer. These results are further quantified through X-Ray reflectivity (XRR) measurements (Figure 1(a)) performed on phospholipid monolayers formed on a surface of water. The obtained electron density profile (Figure 1(b)) depicts the changes of monolayer structure in the resolution of a few angstroms. It can be readily concluded that electrostatic and hydrophobic interactions combinedly govern the assembly of graphene-based materials in and around a phospholipid layer.

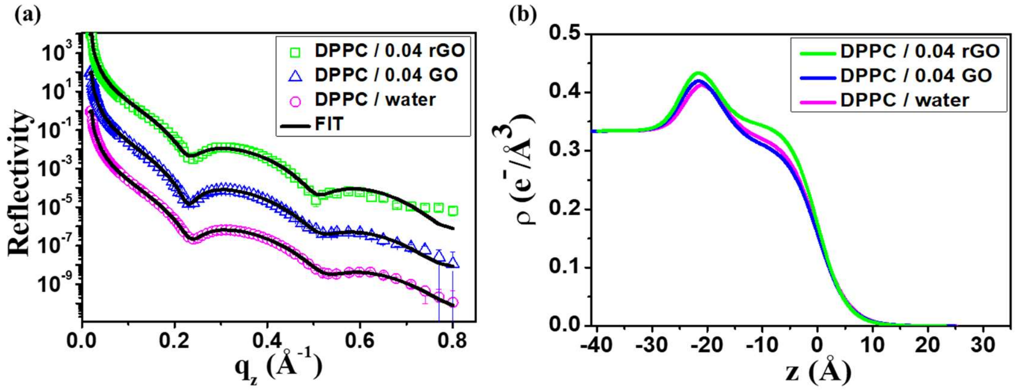

Figure 1. (a) XRR profiles of a phospholipid monolayer at air−water, air−GO aqueous and air-rGO interface at a surface pressure of 30 mN/m. (b) Corresponding electron density profile obtained by fitting the XRR profiles as shown in (a).

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SM-P3

Modified structure and physical properties of a model lipid membrane caused by an Antidepressant Drug

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Amitriptyline (AMT) is a class of tricyclic antidepressants used to treat the symptoms of depression, anxiety, and severe nerve damage [1]. The use of antidepressants has been increasing in the current era. However, little is known about the mechanism of their functioning. There are predictions that their interactions with the cellular membrane and the corresponding altered structure of the membrane play a critical role in the process [2]. The hypothesize is that the drug reduces the reabsorption of serotonin in the plasma membrane, ensuring good mental balance [3]. The present study aims to quantify the effect of this AMT on the structural integrity of the lipid model membrane. Our surface pressure-area isotherm measurements on the sphingomyelin monolayer suggest the increase in the mean molecular area along with the reduced elasticity of the lipid layer (Figure 1). The in-plane rheological measurements follow a similar trend to the static elasticity at both the liquid extended and liquid collapsed phase of the monolayer. The small angle X-ray scattering from the multi-lamellar vesicles quantifies the modified structure of the membrane in a few Angstrom length scales caused by the presence of AMT.

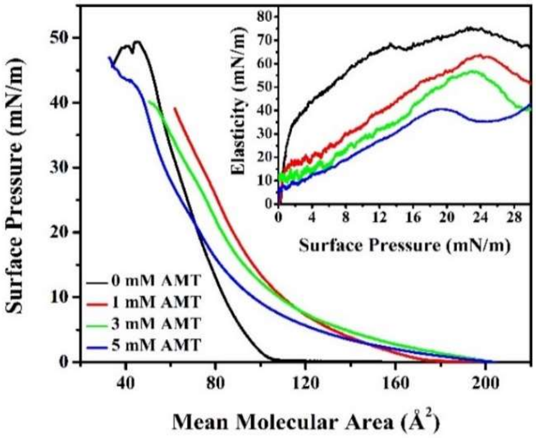

Figure 1: Surface pressure-area isotherm of sphingomyelin lipid monolayer with added Amitriptyline. The inset exhibits the corresponding in-plane elasticity of the lipid film.

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Computational Microscopy of Cyclodextrins - Membrane Interactions

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Cyclodextrins (CDs), cyclic oligosaccharides of α-glucose units, have been used in the pharmaceutical industry as small- and medium-sized drug carriers. The derivatives of βCD (CD having seven glucose monomers) are most widely used due to their efficient production and greater control over the solubility upon substitutions at the hydroxyl groups. Methyl substituted βCDs (MBCD) have been a part of many experimental and clinical studies for their ability to sequester cholesterol from cellular membranes [1-2]. Computational studies have proposed the energetically favourable pathway of cholesterol extraction from its monolayer and lipid disordered regions of membrane bilayer by βCD [3]. However, no exact mechanism is reported on how CDs remove cholesterol and its consequences on the membrane dynamics and CD conformation. Exploring the interactions of CDs with membrane components of the model membrane will help us understand the same in the natural membrane. So, this study intends to analyse the interactions of βCD and its methyl derivatives - MBCDs in the POPC bilayer, with and without cholesterol, using molecular dynamic simulations. The potential of mean force from umbrella sampling simulations is being used to evaluate the energetics of interactions of CDs with membrane components. The effect of different degrees of methyl substitutions and associated conformal dynamics of βCD on membrane fluidity will be discussed. Knowledge of the interactions of MBCD with the model membrane will play a significant role in its successful application in healing cholesterol-enriching diseases like atherosclerosis, Niemann-Pick type C, etc.

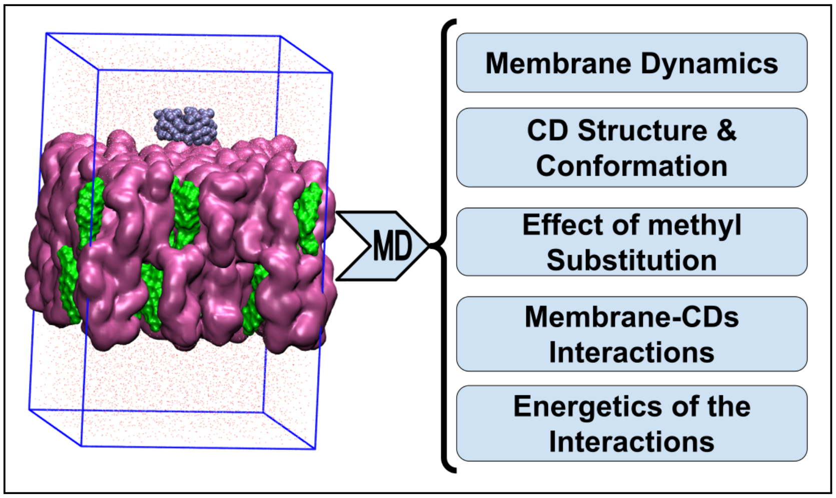

Figure 1: Graphical abstract.
System Description: βCD (purple) in POPC (pink) membrane with 30 mol% Cholesterol (green).

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Influence of SAM Growth on Wetting: Insights from Mass-Transfer Models

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The formation and growth of self-assembled monolayers (SAMs) composed of amphiphiles [1] have gained significant attention due to their diverse technical applications. This work focuses on molecular dynamics simulations results aimed at elucidating the intricate relationship between the wetting behavior of amphiphiles, specifically n-alkanols, and the growth of their SAMs on a mica surface under varying temperature conditions. The investigation quantifies the structural characteristics of the formed SAMs, including density profiles, in-plane radial distribution functions, order parameters, and end-to-end length distributions of n-alkanol molecules within the SAM. Thermodynamic properties such as the second virial coefficient and excess entropy are examined in relation to temperature and time. The growth of the SAM is assessed by analyzing characteristic time scales at different temperatures, in-plane diffusion of n-alkanol molecules, and utilizing classical theories of mass transfer [2] to quantify the growth rate as a function of temperature. These results are then correlated with changes in contact angle and spreading coefficient of n-alkanol droplets on the mica surface over time, providing insights into the impact of SAM growth on the wetting behavior and the mass transfer model of such systems.

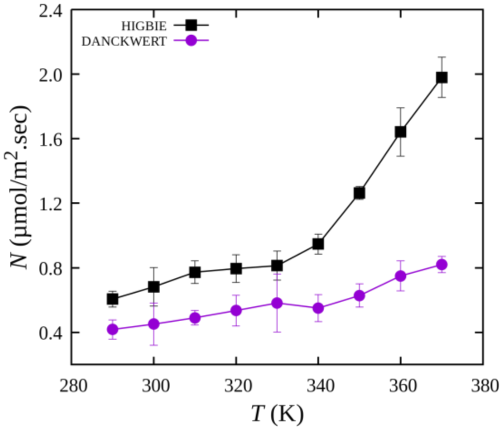

Figure 1: Change in SAM growth rate with temperature.

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Aggregation of chlorophylls on plant thylakoid membranes using coarse-grained simulations

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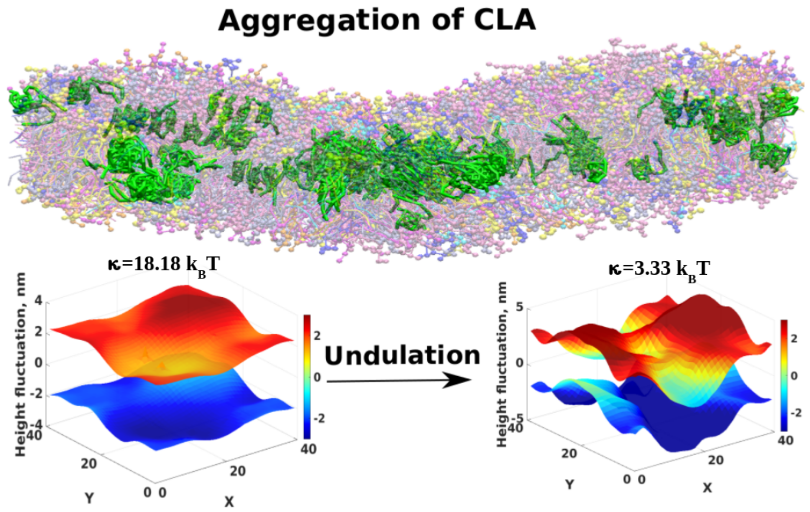
Chlorophyll is an essential pigment in the light-harvesting complex (LHCII), which during photosynthesis, acts as the antennae to capture energy from sunlight and transfer it to the photosynthetic reaction canter. Coarse-grained molecular dynamics simulations of chlorophyll-a molecules (CLA) are carried out in the plant thylakoid membranes with various lipid compositions at 293 K by varying the total lipid: CLA ratio where the bonded potentials of the CLA are derived from Boltzmann inverted canonical distribution[1]. The MARTINI force fields [2] are used for the lipids and non-bonded potentials of CLA. Our simulations show that CLA molecules dynamically form aggregates that break and reform. The lifetime of the dimer and the waiting time of the dimer formation follow bi-exponential distributions for the higher concentrations of CLA. The number of aggregates increases with an increasing concentration of CLA, where van der Waals interactions govern the aggregation. Our simulation confirms that the two most abundant lipids, MGDG and DGDG, that have a strong preference for the vicinity of the LHCII [3], promote the formation of larger chlorophyll aggregate in the plant thylakoid membrane. Preferential locations of lipids near the aggregated CLA results in increasing lateral heterogeneity in the order parameter and density with increasing CLA concentration. This induces more undulations in membranes, resulting in a lower bending modulus and area compressibility. Our work unfolds the mechanism of the formation of CLA aggregates and their effect on the structure of thylakoid bilayers.



Higher number of aggregates, induces higher undulation of the bilayer

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SM-P7

Electroporated-deformation of vesicles under ms-pulsed electric field

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Under electric field, vesicles may exhibit electroporation, a fascinating process that augments the permeability of the vesicle membrane. While the experimental studies have demonstrated tremendous controllability over electroporation under various electric pulses, reported theoretical models largely fail to provide sufficient insights into the experimental results. In the present study, we propose an improved theoretical formalism that can predict pore evolution and consequent vesicle deformation under millisecond-long electric pulses. The novelty of our study lies in modeling the growth of large pores and the current passing through them. Implementing the above, we illustrate that the nature of electric pulses and electrical conductivities plays a vital role in governing the electroporated-vesicle-deformation. The transients captured by our model agree well with earlier experiment findings [1].

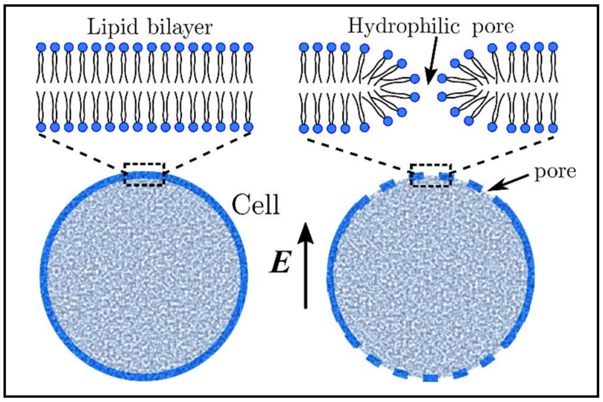

Figure 1: Schematic representation of vesicle electroporation.

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SM-P8

Probing mechanism of membrane activity for small molecule based sequence defined oligomers

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Antimicrobial peptides(AMPs) exhibit excellent potency against bacteria but they are facing challenges due to their susceptibility to proteolysis and toxicity. Towards this, researchers have developed synthetic amino acid-based short peptides where the feature of the host peptides is incorporated [1]. The application of synthetic AMPs is limited due to the high cost of preparation, poor pharmacokinetics and a limited number of genetically coded amino acids to incorporate different functionalities. Therefore, to accommodate the different functionalities and to resolve these limitations, a class of SDMs, namely, the Sequence-Defined Oligomers (SDOs) have been proposed. In SDOs, the sequence of the monomer is precisely controlled on an abiotic backbone. This backbone protects it from enzymatic degradation and facilitates tunable cationic/hydrophobic properties by the sequential addition of monomers having different side chains.

A library of SDOs (**Dec, Oct, Hex, Bnz**) having different hydrophobicity with optimum effect and selectivity has been created recently. SDOs are small molecules and don’t possess any helical segments as compared to AMPs. Apart from these large differences in structure, our preliminary investigation confirms that AMPs and SDOs exhibit similar modes of action i.e., pore-formation and membrane disruptions. The concentrations at which 90% vesicle disruption observed is close to the Minimum inhibitory concentrations (MIC) obtained from bacterial broth microdilution assay of the respective SDOs for B. subtilis. It can be concluded that ‘**Dec’** and ‘**Oct’** SDOs emerged as having the best antibacterial activity among others (**Hex, Bnz, But**). Out of which **Dec, Oct, Hex, Bnz** SDOs shows the membrane disruptions and ‘**But’** SDO shows the pore-formation as a mode of action for their antibacterial activity.

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SM-P9

Techniques for Low temperature Demulsification of Pickering Emulsion

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We discuss the strategies for demulsification of a Pickering-stabilised crude oil emulsion. Pickering stabilisation of a crude oil emulsion occurs when the wax content of the crude oil is high. The wax crystallises onto the interface of the oil and water droplets, while the crude oil flows from the well to the platform through the low-temperature seabed, where the wax gets cooled well below the wax appearance temperature. The wax, while precipitating out, picks up resins and/or asphaltenes, which impart a certain degree of amphiphilicity, which in turn allows the wax particles to grow at the oil-water interface around the water droplets. This leads to the formation of highly stable water-in-crude oil emulsions.

In order to demulsify, the wax shell needs to be broken and then displaced from the interface to either of the bulk phases. This requires a combination of surfactants that can modify the three-phase contact angle of the wax-oil-water interface and also induce phase inversion. We have patented a combination of chemical demulsifiers for low-temperature demulsification of waxy crude oil Pickering emulsions, where "low temperature" implies all temperatures above the pour point of the emulsion and up to 10°C below the pour point of the emulsion.

Our strategy for selecting surfactants involves the measurement of three-phase contact angles to determine the best combination of surfactants. Three-phase contact angle of a water drop placed between the interface of dehydrated crude oil and a horizontal plane surface of wax embedded with resins is observed using a NIR light source and NIR camera.

We also study the interfacial rheological characteristics of the crude oil emulsion with respect to the addition of the surfactants using du Noüy ring. The rheological characteristics, namely the storage modulus and loss modulus of the interface, will allow us to determine the strength of the Pickering shell and hence assess the effect of the surfactants in demulsification.

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SM-P10

Nisin-lipid bilayer interactions: A study on the kinetics of pore formation in vesicle membrane

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Many antimicrobial peptides (AMPs) kill the microbes by forming pores on their membrane. The mechanism of membrane pore formation due to the interaction between AMP and lipid bilayer membrane is of great interest to understand the antibacterial activities of AMPs and for the technological applications involving vesicles. We have used giant unilamellar vesicles (GUV) to study the kinetics of pore formation using the AMP nisin. The GUVs enclosing a fluorescent dye are used to study the pore formation using fluorescence microscopy. The change in the dye concentration in the GUV was obtained from the decrease in intensity of the vesicle due to diffusion of dye molecules through the pores. We have proposed an analytical equation to explain this decrease in intensity. Our equation fits well with the experimental data. The dependence of kinetics of pore formation on the composition of GUV membrane and nisin concentration will also be discussed.

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Spreading and Imbibition of Structured fluids on Porous Substrates

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The spreading and imbibition behaviour of structured fluids on porous substrates is necessary to understand, as they are involved in numerous industrial applications and real-life engineering problems. Studies on drop spreading on a solid substrate are quite common. Drop spreading of complex fluids on solid substrates and Newtonian fluids on porous substrates are available in the literature. But the kinetics of structured fluid drop spreading on porous substrates has not been explored at all. This work investigates the dynamics of the yield stress and shear thinning fluid drop spreading on different porous media of similar pore sizes with different wettability.

Drop diameter and drop height as a function of time have been recorded for different porous substrates and fluid combinations to understand the spreading and imbibition dynamics. From experimental results, the spreading and imbibition behaviour of every fluid-substrate combination has been categorized, analysed and understood. Literature based model was used to compare with the experimental results.

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Indian Society of Rheology

SM-P14

Abstract Title

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Electrodeformation and dye leakage study of Giant Unilamellar vesicles (GUVs) under DC and AC electric field Pulses

The GUVs are micrometers sized vesicles made up of lipid bilayers. The exterior and interior of the GUVs are filled with the liquid solution. The micrometers size and formation with lipid bilayers, makes a GUVs right choice as a bio mimic cell. To explore the fundamentals mechanisms of electroporation and electrodeformation of cells membrane, the GUVs are best choice to know the physics behind all these mechanisms.

When a GUV is subjected to electric field it deforms. The shape deformation of the GUVs depends on whether the applied field is AC or a DC field. Apart from this, factors such as ratio of the internal and outer conductivity of the solution (α), electric pulse duration, electric pulse amplitude, types of GUVs (charged and uncharged) also affect the deformation. Our experiments on GUVs under pulsed DC fields indicates that when the value of the conductivity ratio of the inner to outer fluid, $\alpha = 1$, the GUVs prefers the prolate shape and shapes deformation shown more at higher electric field amplitude. However, when $\alpha > 1$, the GUVs gets deformed more into prolate shape and almost spindle types shapes are also formed. On the other hand, oblate shapes are seen when $\alpha < 1$, means the oblate shapes formation is due to compressive electric forces applied at the equator of the GUVs. The range of electric field amplitude and pulse duration is investigated to know not only the shape deformation but study the reversible and irreversible electroporation of the GUVs. The reduction in the volume of the GUVs after PEF treatment shows loss of volume from inside of the GUV, indicating pore formation in lipid bilayers. To study the size and standing time of the pores, the fluorescence dye filled vesicles analyzed for dye leakage study. The kinetics of the dye release is correlated with the dynamics of the pore formation in lipid bilayer. On the other hand, GUVs that burst show irreversible electroporation. Our analysis indicates that the formation of microscopic structures in such vesicles, are long lived, even after the pulse is switched off, and depend sensitively on the size and strength of the pulse. In this particular study, the pulse width was changed from 100 microseconds to 1 ms and electric field strength was altered from a value of 0.2 kV/cm to 5 kV/cm. The amount and variety of microstructures generated in the vesicle increases when the pulse width and the strength of the electric field is increased.

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Structure and Dynamics of Polymer Tethered Nanocomposites in Bulk and Interfaces

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Molecular simulation investigations on the behavior of hairy nanoparticles (HNPs) with varying interaction energies were conducted. The HNP's consist of a core and 30 chains rigidly attached to the core, and the study focuses on their structural transitions, dynamics, viscosity, and wetting behavior. The results demonstrate that as the interaction energy between the chains increases, the HNP's undergo transitions from disoriented structures to extended and dispersed structures to more organized configurations. Diffusivity measurements along the chains show that the midpoint and endpoint exhibit different mobility at different interaction energy levels. Moreover, the viscosity of the bulk fluid containing HNPs increases with higher interaction energies, indicating more resistance to flow. The wetting behavior of droplets containing HNP's was investigated using contact angle, and interaction energy between chains is kept constant, and interaction energy between the bulk of HNP and the surface is varied. These findings deepen our understanding of HNPs' behavior and properties, offering insights into their potential applications in various fields such as materials science and nanotechnology

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Understanding electrostimulation of neurons without electroporation

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Electrostimulation of excitable cells via Nanosecond Pulse Electric Field (nsPEF) has shown promise in the treatment modality of several neurological disorders, and heart-related diseases[1]. One caveat to this mode of treatment is the possible injury to the cells that are being subjected to the intense electric field, is the unwanted pore formations, leading to the loss of resting membrane potential, rendering the cells unexcitable. Literature suggest that there should be safe gap between the thresholds of excitation and electroporation but the gap size keeps on reducing as we shorten the pulse duration[2]. In the current work, we look at this interplay of electroexcitation and electrporation. We have also looked at the efficacy of compression MHz burst of nsPEFs in electrostimulation without electroporation.

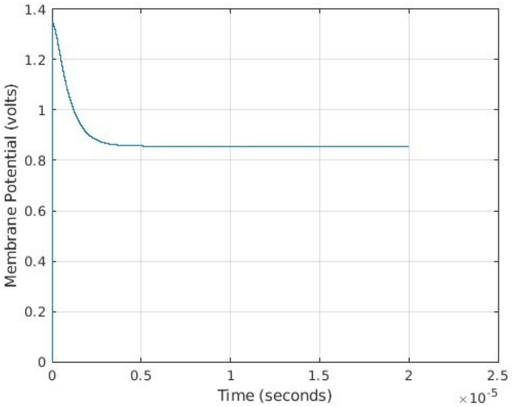

Figure 1: Membrane potential dynamics when 1.35 volts potential being applied to the cell.

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Interactions between similarly charged surfactants & nanoparticles – effect of size and geometry

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The interactions between ionic surfactants and nanoparticles are complex and highly dependent on their charge. In oppositely charged surfactant-nanoparticle systems it is well established that the particle wettability gets modified. Although there have been several studies on binary mixtures of similarly charged surfactant-nanoparticle system, fundamental understanding nature of surfactant-particle association remains poor and often ambiguous. In this study we aim to provide insights into the interactions between similarly charged surfactants and silica nanoparticles and see the overall effect on the surfactant self-assembly. Apart from surface charge, we also study the effect of particle concentration, size, and geometry which influences the anchoring of surfactant molecules on the particle surface by measuring size, zeta potential, conductivity and surface tension measurements as primary parameters. Fluorescence spectroscopy is also used to study some important attributes of the surfactant in the presence of charged nanoparticles.

Keywords: ionic surfactant, nanoparticle, surface tension

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Effect of Dissolved Polymer and Surfactant on the Evaporation of a Liquid Bridge

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Liquid present in the confined regions formed between solids called a liquid bridge, causes capillary forces which will significantly influence the adhesive forces between the solids [1]. In the case of liquids with dissolved solids such as polymers, the viscous forces and the associated non-Newtonian nature becomes significant. Evaporation of the liquid forming the bridge, or a volatile component of a solution leads to neck formation at the center and continuous thinning of it. In stages close to rupture the bridge neck becomes slender and involves a strong extensional flow which can be studied to estimate the extensional viscosity of the liquid [2]. In liquids with laden solids such as surfactants the effect of transient change in the concentration, and consequent change in the liquid surface tension will significantly influence the evolution of the liquid bridge due to evaporation. In this work, we present the experimental study on the evaporation process and evolution of force of a liquid bridge with presence of a dissolved polymer and a surfactant. We considered aqueous solutions of Polyacrylamide (PAM) of concentrations: 25 ppm, 250 ppm, and 1000 ppm. For study on the effect of surfactant, we considered DI water laden with following surfactants, Cetyl Trimethyl Bromide (CTAB), and Sodium Dodecyl Sulphate (SDS). We considered concentrations relative to the critical micelle concentration (CMC) of the surfactants.

In case of PAM solutions, we have observed two regimes in the neck radius evolution of the liquid bridge namely, Evaporation-driven thinning and the Visco-capillary thinning. The latter is the stage close to rupture where viscous forces dominate the evaporation process. The evaporation-driven thinning stage is observed to be similar for the considered concentrations. However, the visco-capillary thinning stage is observed to be more gradual with increase in concentration. This is because of the relatively higher viscous forces of PAM solutions at those concentrations. More work is being carried out on this stage to study the extensional viscosity of the PAM solutions. In case of surfactants, work is being carried out at very low concentrations (0.5 to 2% of CMC) to study the effect of presence of surfactant molecules without any change in the surface tension and high concentrations (50% to 1000% of CMC) to study the effects associated with the variation of the surface tension and formation of micelles with change in concentration as liquid evaporates.

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Flexible Thermoelectric Films Produced via Printing for Energy Harvesting Applications

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Renewable thermoelectric (TE) technologies garnered significant attention due to their environmentally friendly energy harvesting capabilities, devoid of any release of harmful gases. If these TE devices can be flexible and adaptable, they offer opportunities for integration into wearable and implantable electronic technologies. Wearable TE devices, capable of bidirectional conversion between body heat and electricity without requiring moving components, are promising. Assessing the effectiveness of these TE devices relies on a dimensionless figure of merit, $ZT = \alpha 2\sigma T/\kappa$, where α is the Seebeck coefficient, σ is the electrical conductivity, κ is the total thermal conductivity, and T is the absolute temperature.

Conducting polymers (CPs) such as PEDOT:PSS, polyaniline (PANI), and polyethylene terephthalate (PET), and their composites are widely explored in the field of flexible TE applications. These CPs, when combined with inorganic materials, harness the advantage of TE properties of the inorganic while benefiting from the low thermal conductivity and flexibility inherent to CPs. In addition, non-conductive polymers like nylon and polyimide are also being investigated in the realm of flexible TE, where one deposits inorganic TE films on flexible substrates. Notably, ink printing has immense potential in the field of flexible TE because of its ease of processing, cost-effectiveness, and scalability. Here we report a cost-effective and scalable method for fabricating high-performance TE films by employing ink printing on a flexible polyimide (PI) substrate. Detailed insights into the remarkable thermoelectric properties of the flexible polymer-based film within the temperature range of 300 to 450K, along with illustrative proof-of-concept applications, will be presented in detail.

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PRODUCTION OF POLYSTYRENE MICROPARTICLES USING GLASS MODULAR MICROFLUIDIC DEVICE (MMFD)

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Disposing non-biodegradable expanded polystyrene (EPS) waste, known for its high volume-to-weight ratio, presents formidable challenges. A sustainable approach involves upcycling EPS waste into valuable products. In this study, we transform EPS waste into polystyrene microparticles, suitable for applications including lateral flow tests, latex agglutination tests, flow cytometry, and so on. Standard techniques such as spray drying and nanoprecipitation yield particles with varied sizes. The production of monodisperse droplet emulsions through microfluidic methods offers tailored functionalities. However, existing microfluidic approaches using PDMS microdevices or glass chips have limitations, such as specific fluid constraints, operational challenges, and limited reusability. In this work, we introduce a novel microfluidic device using removable capillaries that addresses these issues, allowing cost-effective fabrication using accessible components (see Figure 1a). Experiments with this device generate microdroplets, solidified via the precipitation method, to produce polystyrene microparticles. A homogeneous polystyrene solution in ethyl acetate acts as the discrete phase fluid, while a water-glycerol-EA mixture serves as the continuous phase. Ethanol is the precipitation solvent. Observed under an optical microscope (Figure 1b), collected ethanol droplets form uniform-sized solid particles measuring 80-90 μm. The microfluidic device developed generates monodisperse emulsions, producing narrow-sized polystyrene microparticles. The results of this study can be extended to the recycling of other polymer wastes by suitably altering the device, device preparation methods, operating conditions, solute-solvent-antisolvent system, and separation techniques.

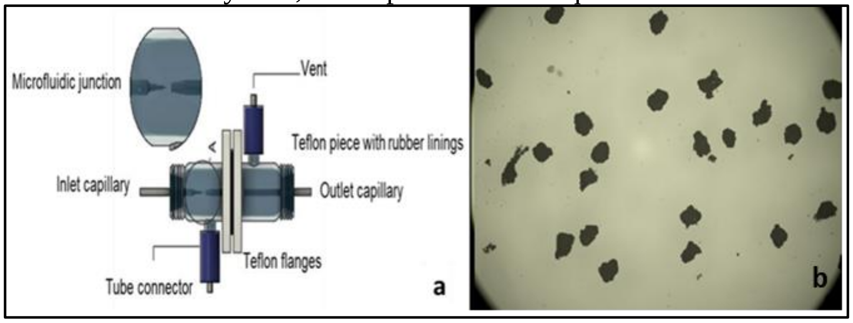

Figure 1: (a) Schematic showing the microfluidic device with the components and the microfluidic junction (b) Microscopic image of the polystyrene microparticles

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Leveraging Stimuli-Responsive and Reconfigurable Block Polymers for Sustainable Materials Design

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Synthesizing reconfigurable nanoscale synthons with predictive control over shape, size, and interparticle interactions is a holy grail for designing stimuli-responsive self-assembled materials. However, grand challenges in their rational design lie in the large space of potential experimental parameters and complex synthetic protocols. More importantly, components commonly used in creating the requisite building blocks are often not biodegradable, making them less favorable amidst growing concerns of sustainability in materials synthesis. Here, we present a strategy for designing complex, reconfigurable building blocks that addresses the above limitations. Our work encompasses two major components. The first involves a joint theory, simulation and experimental study to predict the self-assembled morphologies for a class of biodegradable and stimuli-responsive PVLA-PEG-PVLA triblock copolymers. The second presents a theoretical framework aimed at functionalizing biodegradable block polymers onto nanoparticles to create building blocks with directional interactions that break the intrinsic geometry of the underlying core. Our theories provide unique insights into nanoscale synthesis, allowing for *a priori* design of complex building blocks that can target novel assemblies for sustainable materials fabrication.

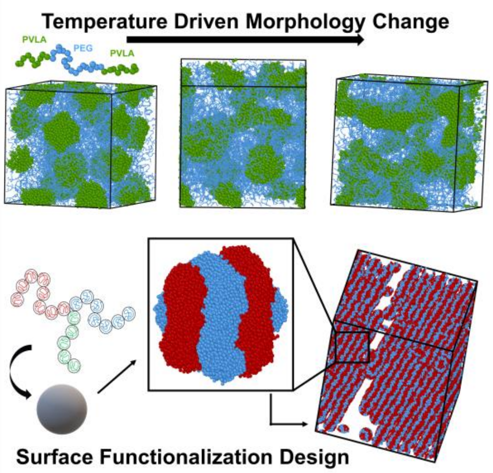

Figure 1. (Top) PVLA-PEG-PVLA temperature driven structural change. (Bottom) Strategy for complex building block design

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Gas transport through amorphous polymer membranes from all-atom molecular dynamics simulations

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Polymers are attractive membrane materials owing to their mechanical robustness and relatively inexpensive fabrication. An important feature central to polymer membrane performance is the distribution of connected void spaces created by inefficient packing of bulky groups on the polymer backbone, known as free volume elements (FVEs). FVEs tend to degrade over time as polymer chains reorganize irreversibly; relating local chain dynamics to the distribution of FVEs can help control phenomena like plasticization and aging. In this work, we use atomistic molecular dynamics simulations to study three polymers - polymethylpentene (PMP), polystyrene (PS), and HAB-6FDA thermally rearranged polymer (TRP). These polymers represent a broad range of structures, allowing us to understand the interplay between polymer chemistry and membrane function. We compute FVEs by identifying filled and free regions in the membrane, as well as atoms that lie on the surface separating the two regions. We find that polymer segments near the surface of voids exhibit faster dynamics compared to bulk segments. This dictates the stability of FVE distribution across different polymer chemistries, serving as a predictor for membrane aging and plasticization. To compute the permeation of gas mixtures such as olefins and paraffins through the membrane matrix, we use the non-equilibrium concentration gradient method. The results from this approach are compared against experimental techniques that measure permeation.

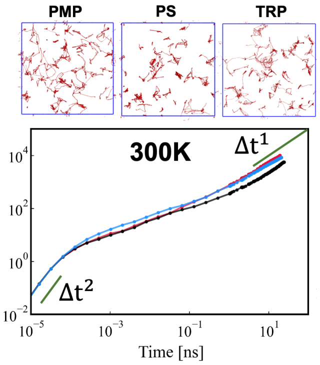

Figure 1: (top) hydrogen dynamics in three polymers considered (bottom) mean-squared displacement of hydrogen through three polymers

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Nanoplastic Formation Mechanisms

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Micro- and nanoplastics (MNPLs) have become a significant topic for study due to their potentially harmful effects on living organisms. As a result, we have a better understanding of the effects of these materials but we still lack a fundamental understanding of why MNPLs form and persist as a result of environmental degradation. In this work we address this topic with the ultimate goal of developing strategies to mitigate their formation. We postulate that the structure of semicrystalline polymers (which make up roughly 70% of the worlds produced polymers) is a key to understanding MNPL formation. In a semicrystalline polymer the degradation is limited to the amorphous regions of the material. These amorphous regions are populated by tie molecules and bridging entanglements which serve as the structural backbone holding neighboring crystalline lamella together. We show that as degradation occurs in the amorphous regions, scission of the tie molecules leads to a breakdown of the polymer and a release of MNPLs. Through modeling of a generic amorphous region with different chain populations we see that the tie chains deplete rapidly as a result of random chain scission. Experimentally we highlight two systems, the first consists of a semicrystalline polystyrene (syndiotatic) and a similar amorphous polystyrene (atactic) which are oxidized using potassium permanganate. Using dynamic light scattering we see that the amorphous polymer shows no particle formation over the observation time period while the semicrystalline material does show the formation of particles, while both polymers show a similar mass loss. The second system we investigate is the degradation of semicrystalline poly(ethylene terephthalate) (PET) using neutral water hydrolysis. In this system we show that despite the very polydisperse products that result from degradation, semicrystalline PET persists through the degradation and leads to nanoscale, ‘platelet’ particles that we can then characterize further using x-ray scattering, light scattering, and calorimetry.

Modeling Compatibilization of Mixed Plastic Wastes

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Most of the industrially used polymers are immiscible and incompatible and do not form a homogeneous mixture. Stabilizing these immiscible mixed plastics could increase their lifespan and enable previously unrecoverable mixed plastic wastes to be reprocessed and reused. Thus, developing new methods for increasing blend compatibility is of increasing demand for sustainable polymer development. Here we study how dynamics covalent bond can reactivate mixed plastic "dead" chains into compatibilized multiblock copolymers. We develop a bead-spring model and carry out molecular dynamics (MD) simulation of an incompatible homopolymer blend, whose constituents are termed A and B. Dynamic crosslinks are created only between pairs of dissimilar (AB) monomers within a predefined cut-off distance. Figure 1A and 1C are with 5% and 15% of AB crosslinked monomers, respectively. The corresponding radial distribution functions for AA, BB and AB pairs are shown in Fig. 1B and 1D. These results illustrate the clear transition from an immiscible blend to a progressively more miscible one. Detailed analysis of the static structure factor shows that the 5% AB crosslinked system is likely microphase separated while the 15% system is completely miscible. Consistent with this conclusion, there is clear evidence of decreased sizes of the A-rich and B-rich domains with increased AB crosslinking. The creation of a "living" gMBCPs, is found to be the underpinning driver for the increased miscibility. In contrast, static crosslinking creates a much less miscible system. We establish correlations between miscibility, lifetime of dynamic crosslinks, the fraction of crosslinks. We show that the universal dynamic crosslinking improves the mechanical properties, and thus the reusability of the blend. Our theoretical prediction is validated by recent experimental studies.

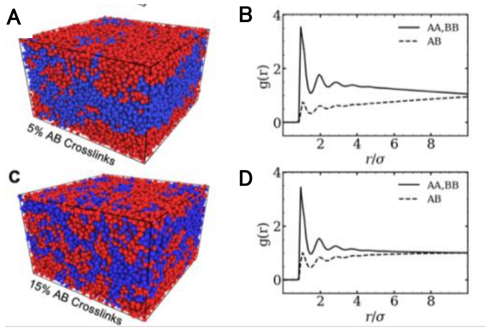

Figure 1: Coarse-Grained MD Simulations of a Binary Polymer Blend. MD snapshots of 5% AB dynamically crosslinked (A), 15% AB dynamically crosslinked blends (C). The corresponding radial distribution functions are shown in (B), and (D), respectively.

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Unprecedented adhesion of polyethylene-grafted sheet-like silsesquioxanes

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Abstract

Polyethylene is one of the most widely used commodity plastics. Since polyethylene is an apolar, semicrystalline polymer, there is interest in the preparation of functional polyethylenes that find use in a variety of applications. For example, polyethylene shows very poor adhesion to most substrates, necessitating the use of tie layers. Here, we report the preparation of a novel nanocomposite comprising polyethylene covalently grafted onto sheet-like silsesquioxanes, with unprecedented adhesion to metal and glass. We measure bonding strength of the order of 100 MPa to stainless steel and aluminum, 10-fold higher than reported even for polyethylene copolymers. The nanocomposite exhibits an increase in the polar component of the surface energy, yet remains compatible and cocrystallizes with a polyethylene matrix. Synthesis of the nanocomposite starts with preparation of a norbornene-grafted layered Mg-silsesquioxane, followed by grafting of second-generation Grubbs catalyst and ring opening metathesis polymerization of cyclooctene. The polycyclooctene is catalytically hydrogenated to yield polyethylene. Detailed characterization at each stage of the synthesis is reported.

Modeling Catalytic Degradation Mechanism of Polymers Using Density Functional Theory

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Most of the industrially used syntheic polymes do not disintegrate in nature. It seriously pollutes the environment. Developing cost effecitive and high fedality pyrolysis to degrade, reprocess and recycle mixed palstic wastes is key for the sustainabilty of the planet. Widely used polymers such as polystyrene (PS), which ranks fourth in the world's production of plastics generates a large portion of "plastic waste" after it's lifecycle [1]. Because PS has persistent chemical characteristics that make it difficult to disintegrate in nature, it seriously pollutes the environment. Also, production of a large number of PS products leads to the waste of resources as it become unusable after its lifecycle is over [2]. Recent research shows degradtion and recovery of PS in catalytic ervironment is an effective way[3]. However, the fundmaental mechanism of degradation is not fully understood. Here, we employ first-principles based Density Functional Theory (DFT) calculations to investigate two catalytic degradation (acidic and alkaline) mechanism of several polymers viz. polystyrene, polymethyle methacrylate, and polypropylene. Optimized geometry of all the structures are obtained. We estimate the thermodynamic and kinetic pathways of the degradtion. We predict the amount of monomer recovers and other byproduct during the degradation. The data shows new insights into the molecular-scale reaction mechanism of polymer degration. This highlights the importance of our method to better understand the reaction mechanism of catalytic degradation of polymers.

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Predicting Percolation Phase Behaviour of Polymer Electrolytes using Coarse-Grained Molecular Simulation

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Polymer electrolytes are of interest for the next generation energy storage devices due to the advantages like high energy density, low weight and non-flammability. They combine the solid-like stability of polymers with the high conductivity of ionic liquids. However, the practical application of polymer electrolytes is dependent on addressing challenges related to the slow dynamics of the polymer matrix and its impact on ion transport[1,2]. Particularly, how ion moieties distribute in a polymer matrix depends on ion concentration, dielectric constant, and ion pair size[3], and its influence over transport properties is an unsolved problem.

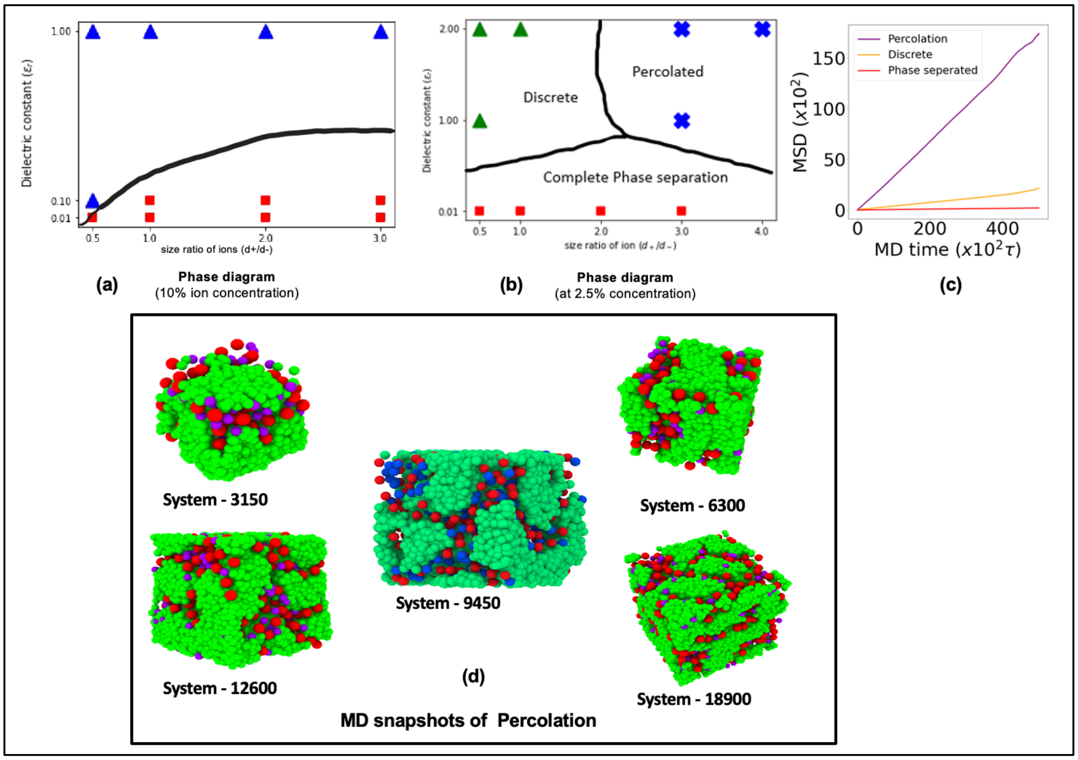

Figure 1: (a–b) Proposed phase diagrams at 10% and 2.5% concentration respectively. The proposed phase diagram(s) is between complete phase separation, discrete and percolation aggregate.(c) Comparison of mean square displacement between all three phases at 2.5% ion concentration. (d). MD snapshots of percolation aggregate at 2.5% ion concentration, ε_r =1, d_+/d_- =3 with variation of system size from 3150 particles to 18900 particles

Here, we conduct coarse-grained molecular dynamics simulations[4] of a phenomenological model to develop a deeper understanding between these factors. Specifically, we study ion solvation and its connection to conductivity in a polymer matrix. We report a range of microstructures as a function of ion size ratio and dielectric constant and propose a new phase diagram for polymer electrolyte. We calculate glass transition temperature, segmental relaxation time, decoupling exponent for percolating structure to establish a relation between them as well as the molecular mechanics for high conductivity. Our work has important implications in next generation solid-state electrolyte design.

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Conductivity of a Size Polydispersed Ionic Liquid: A Molecular Dynamics Simulation Study

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A size polydispersed ionic liquid (IL) corresponds to an ionic liquid mixture with a large number of components. Mixtures offer a unique way to tune the properties of IL besides changing the cation/anion pairing. Although studies on IL mixtures are carried out, they are confined to 2 or 3 components of pure IL;[1,2] and a large amount of studies are on mixture with other solvents. In this study, we performed molecular dynamics simulation using coarse-grained spheres with varying diameters representing a size-polydispersed IL system. The size of cations follows Gaussian distribution, representing an n-component mixture. Using this model, the response of the system's conductivity on varying degree of size polydispersity is studied in detail. From this study we found a non-monotonic dependence of conductivity on degree of polydispsersity.

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Development of Polymer/Composite based Growing Chamber with Controlled Temperature for Soil-less Agritech

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Soil-less agritech is a method of growing plants in any medium other than soil, such as air, water, etc. Soil-less system techniques have been integrated into horticulture production to maximize the efficiency in the use of water and nutrients [1]. In soil-less farming, the major task is to control and maintain environmental conditions such as temperature, relative humidity, dissolved oxygen, and nutrition uptake quality [2]. The root zone temperature affects the growth of the plant. As the temperature increases the concentration of dissolved oxygen in water decreases[1] The desired concentration of dissolved oxygen in water for plants to grow without stress is 7.7 mg/l. Temperatures above 30 °C are not favorable for most Indian crops[2]. To overcome this problem growing chambers of polymer composites are being developed for thermal regulation in soilless agritech. This may be achieved by modulating the thermal conductivity and the radiation reflectivity of the materials that make a growing chamber. Phase change materials may also be used in the chambers to keep the temperature in the desired range (20-26 °C) [5].

In this study, growing chambers were made using composites of HDPE or LLDPE with fillers such as clay particles or marble dust. Composites were fabricated by injection molding. The melt flow behavior of polymer melt was investigated using a melt flow index (MFI) tester. The MFI values of HDPE composite samples are significantly higher than those for LLDPE composite samples due to the higher density of HDPE. As the clay particle loading increases up to 30% (w/w), the MFI remains relatively unchanged. By using the Hagen-Poiseuille equation, it shows that MFI is directly proportional to density and inversely proportional to viscosity as shown in equation (1).

$$\mathrm{MFI} = Q^{*}\rho = \frac{\rho\pi\Delta P R^4}{8\mu L} \qquad \ldots\ldots(1)$$

$$\mathrm{MFI} = K(\rho/\mu), \text{ where } K = \frac{\pi\Delta P R^4}{8L}$$

K is a constant
Q = volumetric flow rate
ρ = density of fluid
ΔP = pressure drop
R = radius of the barrel
μ = viscosity of fluid

Polymeric chambers help in keeping the temperature low as compared to surroundings for a reasonable duration. It is observed that composite chambers with filler particles, loadings up to 30 wt.%, do not offer any advantage, as compared to a chamber made up of 100% LLDPE, in terms of lowering the water temperature as shown in Figure 1.

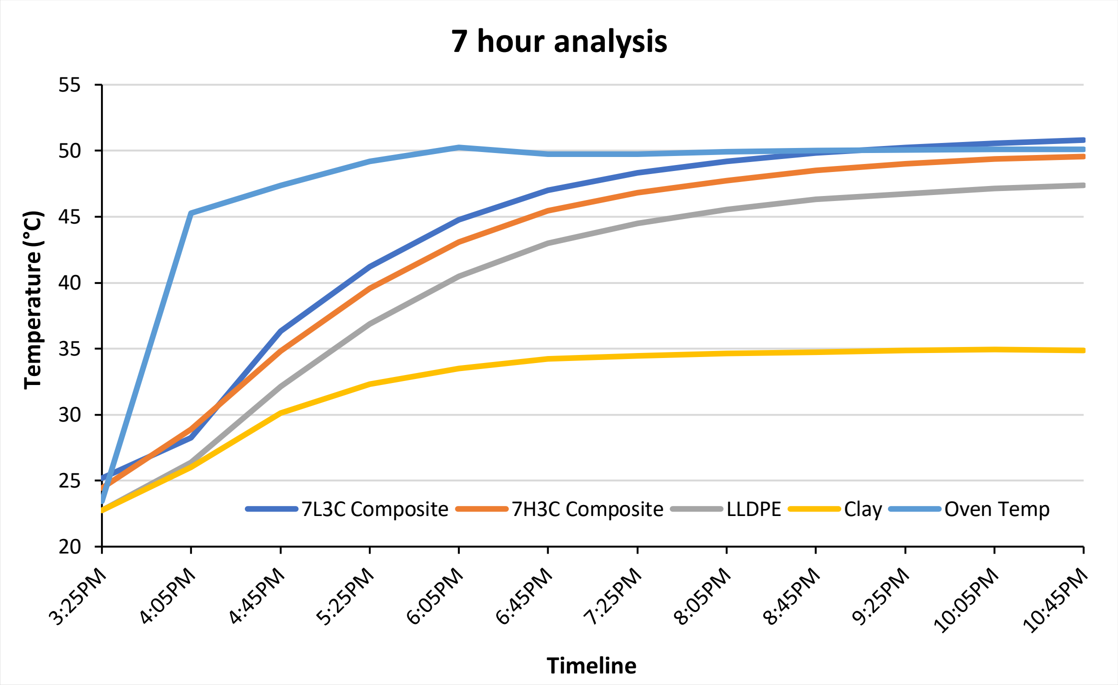

Figure 1: Temperature vs time plots for various growing chambers

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Investigating the Chaperone Mechanism of α-Crystallin in Preventing γD- Crystallin Aggregation in Cataract Formation

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Cataract, a leading cause of global blindness [1], arises due to the aggregation of crystallin proteins within the eye lens, leading to opacification and loss of transparency. Although present at a high concentration of up to 450 mg/ml, crystallin proteins remain soluble, maintaining lens transparency and the refractive index [2]. Chaperone proteins, particularly α-crystallin, play a vital role in preventing the aggregation of these proteins [3]. However, the specific molecular interactions between α-crystallin and other crystallin subtypes, such as γD-crystallin, which is one of the most abundant crystallins in the human eye lens, remain poorly understood.

In this study, we aimed to elucidate the interactions between the α-crystallin's ACD [4] domain and the domains of γD-crystallin. To achieve this, we employed a multifaceted approach combining molecular docking, interaction studies, molecular dynamics simulations, and Markov state modeling-based free energy calculations. Through molecular docking studies, we first probed the binding affinity and specificity of the ACD domain with the domains of γD-crystallin. Subsequently, we conducted detailed interaction studies to gain insights into the key residues and molecular forces driving the stable complex formation. To quantify the thermodynamic stability of the α-crystallin-γD-complex, we calculated the free energy of binding, comparing it to the stability of γD-crystallin in the absence of ACD. Our findings shed light on the energy landscape and the role of the ACD domain in mitigating the aggregation process of γD- crystallin, a crucial step in cataract formation. Furthermore, we harnessed molecular dynamics simulations to explore the dynamic behavior of the ACD-γD complex over extended time scales. These simulations allowed us to investigate the conformational changes and fluctuations occurring within the complex and provided valuable insights into its overall stability.

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Designing functional electrospun matrices: from polymer physics to biomedical applications

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Our lab is broadly interested in studying structure-property-processing relationships in polymeric biomaterials with the goal of developing soft materials for biomedical applications. Our major focus is the process of polymer electrospinning, a technique used for the preparation of fibrous non-woven meshes. We investigate electrospinning via direct in situ visualization of the electrified cone/jet to gain insights into jet initiation/stretching, as well as the roles of specific system/operating parameters that dictate fiber formation. Using these insights, we develop fibrous meshes with predictable diameter and specific mesh properties. The primary application of such meshes in our laboratory is in controlled drug/protein release. Here, we are interested in understanding dominant matrix factors that control drug release to design electrospun-based carriers that exhibit controlled and sustained release of immunomodulatory drugs. We also develop new technologies to simultaneously deliver multiple drugs and cytokines while retaining independent control over release and preserving conformation/function. In close collaboration with biologists, we deploy such materials to target dysfunctional immune responses associated with degenerative diseases. A recent interest in our group is the development of co-amorphous drug formulations, wherein we are particularly interested in uncovering rules governing the physical stability of such systems.

Keyword: Electrospun polymeric biomaterials

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Proteins, Strings, and Mechanisms

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Our research group works primarily on proteins, the molecular machines that drive the majority of cellular processes. We explore in great detail the how and why of protein folding, i.e. the mechanisms driving the linear string of amino residues folding into intricate three-dimensional structures, the choreography of various residues involved (dynamics), the imprints of function on structure, and ways to engineer them. By combining experiments, simulations, and theoretical modelling, we study an array of emergent behaviors including cooperativity, allostery, higher-order assembly and phase separation, with implications in disease origins, cellular signaling and stress response mechanisms.

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Tracing Solvent Hydrogen Bond Network Reveals Surprising Facts

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Hydrophobicity is believed to drive many biophysical processes such as protein folding, conformational changes, and association of macromolecules. Yet, the solvent interaction usually gains less attention compared to the macromolecule in the system. Tracking the solvent properties, however, reveals many interesting characteristics of biophysical processes. In this table talk, I would like to discuss some such interesting and counterintuitive results such as hydrogen bonding with peptides lead to entropy loss for water, self-assembly of peptides is not a hydrophobic collapse, water confined in the cyclodextrin cavity possess high entropy compared to bulk water but are only enthalpically frustrated. I will also demonstrate that many interactions in aqueous solution are strongly correlated to the hydrogen bonding.

Keywords: Hydration Thermodynamics, Hydrogen Bond Network.

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Homocitrulline-containing peptide amphiphiles: Amyloids or Coacervates?

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The term "Amyloids" is typically associated with debilitating diseases such as Alzheimer's (AD) and Parkinson's (PD). However, there are numerous examples of naturally occurring benign functional amyloids such as curli protein, silk proteins, chaplins, sup35 and CPEB. The extreme stability of the amyloid structures owing to the presence of an extensive beta sheets network, has inspired many to develop robust mutipurpose biomaterials.

In our laboratory, recently, we have discovered that lysine-based charged neutralizing post-translational modifications such as carbamylation and acetylation are a strong driver of amyloid formation and can convert an unsuspecting lysine-rich peptide sequence to an aggregation hot spot. We have utilized this observation to create a new class of homocitrulline (or carbamylated lysine) containing peptide amphiphiles, which self-assemble into multifaceted scaffolds with diverse functionality.

In a systematic study, we assembled oligo lysines (3K,5K, and 8K) and then capped their N-terminal ends with aliphatic chains of varying lengths, such as acetic acid, hexanoic acid, and nonanoic acids. Thus, prepared amphiphiles were water soluble and showed no aggregation or self-assembly. However, when carbamylated in situ to generate homocitrulline, they readily self-assembled into fibrillar structures, with the rate of assembly and structural features being highly dependent on the lysine numbers and hydrophobic tail length. The same amyloids, when melted in acid and exposed to water, exhibited liquid-liquid phase separation and led to the formation of stable coacervates. We have further demonstrated that fibrils could be used as the absorbant for water-soluble hydrophilic dyes, and coacervates can be loaded with therapeutic drug molecules for efficient delivery.

In summary, we have discovered a new methodology to prepare a range of peptide-based amphiphiles where self-assembly is primarily driven by Hydrogen bonding, and the same peptide amphiphiles can be used to form at least two distinct classes of self-assembled structures. While amyloids could be used to form hydrogel or structural scaffolds, coacervates could be tuned to control release and targeted drug delivery applications.

Keywords: Amyloids, Peptides, Amphiphiles, homocitrulline, aggregation.

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Efficiency of an Active Brownian particle in a ratchet potential

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In this work, we study the energetics of an active Brownian particle [1] in a piece-wise linear ratchet potential subjected to a load as characterized by the energy input, power output, heat dissipated and the efficiency of the motor. There are optimal values of various parameters such as the self-propelled velocity, temperature, asymmetry of the potential, at which the efficiency attains a maximum. Efficiencies greater than 10% are observed as a function of several parameters.

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Towards developing sustainable fat substitutes

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Sustainable and healthy diets are meant to satisfy the needs of the present generations without compromising on environmental resources or biodiversity but in turn be affordable and nutritious. This study is focused towards developing healthy vegan fat substitutes by analysing rheological properties, texture and microstructure of sustainable fat substitutes. We systematically develop an emulgel, oleogel and hydrogel from plant sources that can be used as basic building block to develop plant-based butter substitutes. We use a combination of structure and texture characterisation to investigate the properties of the pure building blocks as well as the properties of the bigel, formed by mixing the oleogel and hydrogel in different proportions.

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Keyword: Food rheology

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A discussion on a few models for Thixotropic fluids

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Thixotropy and associated behavior have attracted modeling interest over the last few decades. Some popular models from the literature such as due to Wagner, Larson and co-workers will be discussed in this work. Strengths and shortcomings of different approaches will be highlighted.

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T2-04

Regulation and role of plasma membrane mechanics in adherent cells

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The plasma membrane's mechanical state is crucial for various cellular processes like trafficking and motility. In the lab we explore mechanisms involved in establishing membrane homeostasis while also studying the role of membrane mechanics in different contexts. We study role of endocytosis and caveolar dynamics in membrane tension regulation. Our experiments also explore how membrane mechanics is involved in collective cell migration of fish keratocytes, cell-cell fusion of myoblasts, and clustering states of signalling receptors. We employ a range of techniques from non-invasive measurements of basal membrane height fluctuations, to Total Internal Reflection Fluorescence (TIRF) Microscopy, and super-resolution microscopy to address these questions.

Keywords: cell membrane homeostasis.

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The FENE-mode model to accurately predict temporal variations of configuration and stress of polymer chains in solutions

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In this study, we formulate a new constitutive model, termed “FENE-mode”, for prediction of conformation and stress of dilute polymer chains in arbitrary flow fields. This is obtained using preaveraged equations of the normal modes, while using a “representative” spring constant that is a simple function the magnitudes of the first and second modes. Note, these modes account for both chain stretch and chain folds, to some extent. Numerical integration of this model is several orders of magnitude faster than Brownian dynamics (BD) simulations of multi-bead-spring chain models. However, the predictions are much more accurate than other preaveraged models proposed earlier. To show this, we compare the predictions of the FENE-mode model with those from BD simulations in startup of uniaxial extension, relaxation after cessation of this flow, steady shear, and mixed flows. For all flows considered, even when few modes are used, we observe much better agreement with BD simulations than those of the existing preaveraged FENE-P and FENE-PM models. The model allows for cost-accuracy trade-offs through appropriate choice of the number of modes and thus should be ideal for multidimensional simulations of polymer flows.

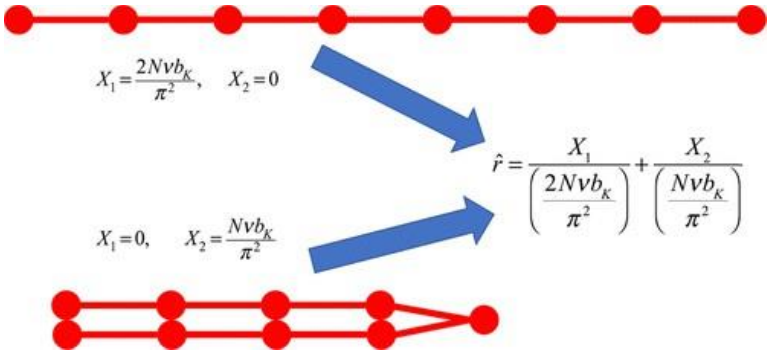

Figure 1: Summary of the contribution of the first two modes to the estimation of the representative spring constant. Note, the first mode reaches a maximum when the chain is fully stretched but the second mode reaches a maximum when the chain is stretched but bent as a hairpin. In either configuration, one mode reaches a maximum while the other one becomes zero.

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Multiphase Flow and Flow in Porous Media for Energy Applications

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Developing a clean, low-carbon and energy efficient process for industrial decarbonization is a main objective of the multiphase flow and porous media research laboratory at IIT Madras. Multiphase flows encountered in various energy fields such as carbon capture and sequestration, as well as various chemical processes. One of the focus areas of this research group is to find out process intensification options for both adsorption-based CO2 capture and absorption-based CO2 capture in terms of new sorbent structures, new sorbent/solvent materials for efficient CO2 absorption/ adsorption capacity and new reactor module for better mixing of gas-solid and gas-liquid flows, which will be discussed in detail in the talk. The multiphase flow transport in the permeable media is another focus area, the group is actively working on and will be discussed in the talk. Multiphase flow through permeable media can be found in many subsurface engineering technologies like oil and gas extraction, CO2 sequestration, and environmental issues like contaminant transport and water resource.

Additionally, the dynamics of three phase catalytic processes will also be discussed in the talk. The yield of the desired chemical product and process efficiency of three phase suspension process bases on various transport processes over a wide spectrum of spatial and temporal scales. An open question on the effect of fluid and particles properties on bubble coalescence and breakup, which affects the hydrodynamic and mass transfer in the three-phase suspension reactor will be discussed in detail in the table talk.

Keyword: Multiphase flow

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Moving Contact Lines: singularity, flow fields, and new insights from experiments

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A moving contact line (MCL) forms when an interface between two immiscible fluids intersects a solid surface, a phenomenon encountered in everyday scenarios such as water drops sliding down a windowpane, spreading paint on drywall, or ink-jet printing. What makes this problem fascinating is the singularity that arises at the moving contact line when the conventional no-slip boundary condition is applied to the moving solid. Most of our understanding of flows near a moving contact line is based on theoretical models in the low Reynolds number and low capillary number limit. A significant portion of experimental work on MCL has primarily focused on elucidating the angle-versus-speed relationship, with limited attention paid to the flow patterns. Following a concise introduction to this classical problem in fluid mechanics and the key outstanding questions to address, I will discuss results from an experimental campaign involving a wide variety of fluid combinations, contact line speeds, and solid wettability. These experiments allow us to test theoretical models rigorously. A common strategy to resolve the contact line singularity is to impose a slip near the MCL. Our experiments offer new insights into how Nature resolves the singularity near the MCL. However, our experiments also pose new challenges to theoretical models in the form of flow fields that directly contradict prevailing theories within certain regions of the parameter space.

More details can be found here: https://arxiv.org/abs/2311.09560

Keywords: Moving Contact Lines, Thin films, Surface tension

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Insights into water-salt dynamics in polyamide and graphene oxide-based membranes and protein-surface interactions via computational approaches

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We will present the results from molecular dynamics simulations on the SAPA membrane in the FO process to understand the structural properties and performance of the membrane at the atomistic level. We used pure water as the feed and Na_2SO_4 as the draw solution. It is observed that the SAPA membrane shows excellent water permeability and no reverse draw solute flux. To further test the dynamics of salt ions inside the membranes, we performed two distinct equilibrium simulations on systems consisting of either monovalent salt, such as NaCl, or divalent salt, such as Na_2SO_4. The atomistic details of the interactions between the functional groups of the membrane and salt ions provided here can inspire further experiments on SAPA membranes in the context of separation of monovalent and divalent salts, which have applications in the treatment of textile industry wastewater.

In the second part, we will present the results on shale gas wastewater (NaCl, $CaCl_2$, and crude oil) treatment with cation (K+, Mg$^{2+)}$ intercalated GO membranes. This study reveals that the presence of a higher concentration of cations inside the GO membrane induces higher water resistance in the membrane. In addition to the concentration of intercalated ions, interlayer distance also plays a significant role in determining water permeance. We also observed a difference in the crude oil aggregate formation (a composition of alkanes, cycloalkanes, and aromatics) in the two systems (more stable aggregate in K^+ ion intercalated GO membrane system as compared to Mg^{2+} ion intercalated GO membrane system) during the forward osmosis (FO) process.

In the third part of the presentation, we focus on protein-surface interaction and protein-paratope interaction. We considered two systems with different counterions (Na^+ and Ca^{2+}), namely Na-MMT and Ca-MMT, to investigate the effect of different ions on S protein-MMT interaction. Structural modification of S protein was observed in the presence of MMT surface, particularly the loss of helical content of S protein. We observed that electrostatic and hydrophobic interactions synergistically govern the S protein-MMT interactions. However, hydrophobic interactions were more pronounced in the Na-MMT system than in Ca-MMT. Molecular mechanism of disaggregation of preformed LS-shaped $A\beta_{42}$ protofibril with a flexible, hairpin-like synthetic paratope (SP) will be presented. Our simulations demonstrate various potential binding sites for SP on $A\beta_{42}$ protofibril. However, binding of SP at the amyloidogenic core region (KLVFF) shows pronounced structural disruption of $A\beta_{42}$ protofibril. Our results show heavy loss of β sheet content, dismantling of K28-A42 salt bridge, and destruction of key contacts in the hydrophobic cores of $A\beta_{42}$ protofibril in the presence of SP.

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T3-04

Soft matter biomicrofluidics – from mimicking blood flows to cancer drug screening

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Over the past few decades, microfluidics has emerged as an extensive and multidisciplinary area of research within the domain of fluid dynamics. The rise in technological advancements especially in the field of electronics and instrumentation has resulted in the development of microfluidics based biomedical devices and techniques for diagnosis, vital monitoring, support systems, and therapeutic screening. Microfluidics comes handy due to its inherent advantages in sensing, sample requirements, time of detection and the affordability to the masses. In the light of these developments in the field of microfluidics with potential applications in areas ranging from soft matter physics to global healthcare, my research was focused on experimental and theoretical aspects of fluid flows in deformable microchannels that mimic the human vasculature. The experimental results, corroborated with theoretical analysis have demonstrated the intricate relationship of the wall deformation and the pressure drop across a deformable microchannel. Later, it was extended to time varying flows and flows of red blood cells in hydrogel based deformable microchannels. Another aspect that would be discussed is the wetting of droplets laden with microparticles and bacteria on highly repellent (superhydrophobic) surfaces. Further, in the fight against cancer, commonly followed microfluidics-based approaches for cancer drug screening are complicated and expensive, that warrant high-end equipment and sophisticated fabrication techniques. We propose a low-cost drug screening and viability testing platform with minimal fabrication requirements. A novel method of tumoroid generation inside a microfluidic environment is introduced that exploits pure hydrodynamic and interfacial effects for the screening of chemotherapy drugs.

Keyword: Bioimicrofluidics

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T3-05

Numerical Modeling of Capsules in Microchannel Flows

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Understanding the dynamics of soft membranes in a fluid flow is important in various biological systems. In this talk, we will discuss numerical formulation for simulating the dynamics of a cluster of capsules subjected to a shear and extensional flow, such as in a microchannel with a constriction. We have developed a parallel numerical solver that employs a front-tracking algorithm in a finite volume method framework to capture the membrane dynamics in three-dimensional flows. An interaction potential is used to model the interactions between the membrane and the walls of the microchannel.

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Modeling multiphase reactors for clean energy

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Multiphase reactors are ubiquitous in the chemical industry and play a central role in the emerging clean energy technologies, such as biomass to biofuel conversion and CO2 capture. The performance of these reactors relies on the coupling between chemistry and multiphase hydrodynamics. Historically, numerous empirical correlations have been developed that are still in use to design these reactors. This strategy is not optimal and requires extensive experimentation at various scales, making the development of a new process expensive and time-consuming. Recent advances in high-performance computing and numerical techniques allow high-fidelity simulations of reacting multiphase flows. These simulations can reduce the reliance on empirical correlations and the number of experiments required. Moreover, combining the high-fidelity data and machine learning algorithms can be used to develop accurate design tools for the emerging technologies utilizing multiphase flows.

Keyword: Multiphase flow

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Understanding the effect of Methyl group of molecules in polymer solutions

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Enhancement of the potency of drug molecules by addition of methyl group is a trade knowledge among pharmacological community. A recent survey shows, almost 70% of the commonly used drugs have one or more methyl groups present in it. The stereochemical effect caused by the methyl group, enhances the binding efficiency and specificity of the drugs and this effect is commonly known as the magic methyl effect. Even though the interest in the structural chemistry of methylated drug/small molecules spans over a decade, the transport properties of such molecules are not well studied. In this work we present a curious result regarding transport property of a small, methylated fluorophore (Rhodamine 6G, R6G) compared to non-methylated fluorophore (6-HEX) in the presence of aqueous solution of polymer (polyethylene oxide, PEO). We find that the diffusivity of the R6G decreases with increase in PEO molecular weight until we reach semi-dilute concentration, like 6-HEX. Above the semi-dilute concentration R6G shows enhancement in diffusivity compared to 6-HEX. This observation was obtained using Fluorescence correlation spectroscopy (FCS). We have independently validated the observation using molecular dynamic simulation (GROMACS), and scaling theory. Based on our simulation and theory we conclude that the effect is mainly due to the hydrophobicity imparted by the methyl-groups. The repulsive interaction doesn't allow R6G to interact with hydrophilic polymers like PEO whereas more hydrophilic molecule 6-HEX has favorable interaction with PEO which slows its diffusive transport. We believe this underling physics will allow a much better design of future drugs.

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Pattern Formation in thin films of evaporating polymeric solutions – an interplay between evaporation and spreading rate

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Evaporation is a recurring phenomenon in everyday life – coffee ring formation, drying of paints – and in various technologies – large-scale coatings, and 3D printing. Despite the apparent practical simplicity, evaporation is inherently a nonequilibrium process involving a complex interplay of various processes including wetting, spreading, diffusion, crystallization, and glass transition. Using a combination of microscopic tools and linear stability analysis, we probe evaporation-induced structure formation in polymer and polymeric nanoparticle solutions. By controlling the evaporation rate and the concentration of the polymeric solutions spread on the water surface, we observe patterns like flat islands, domains, and networks suggesting dewetting of solutions at the air-water interface. Intriguingly, we reveal a non-monotonous variation in the height and the lateral length scale of the patterns with solution concentration and the evaporation rate of the solvents. We argue that an interplay of the rates of spreading, and evaporation may underlie the observed non-monotonous variations in the relevant length scales.

Keywords: Structure Formation, Evaporation, Polymer Layers

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Polymers for Advanced and Sustainable Manufacturing

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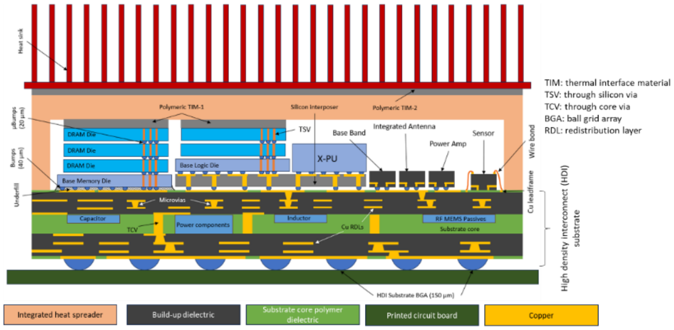

Figure 1: A high density interconnect substrate demonstrating the role of polymers in electronic packaging.

Dr. Deepak Arora is a faculty with the department of Chemical Engineering at IIT Jodhpur. He has a Ph.D. and M.S. in Polymer Science & Engineering from University of Massachusetts Amherst. He has a BTech Dual Degree in Chemical Engineering from IIT Madras.

His industrial experience is in the domain of material, process, and technology development for electronic packaging of semiconductor devices while working with Intel Corporation and Fujifilm Electronic Materials. Current research, at IIT Jodhpur, is focused on the development of novel polymeric formulations and composites for semiconductor packaging, advanced manufacturing and agritech. Objective of this table talk is to further these areas of research through collaborating in these domains and learning about relevant future challenges and opportunities via interacting with faculties, industry professionals, students, and potential PhD candidates.

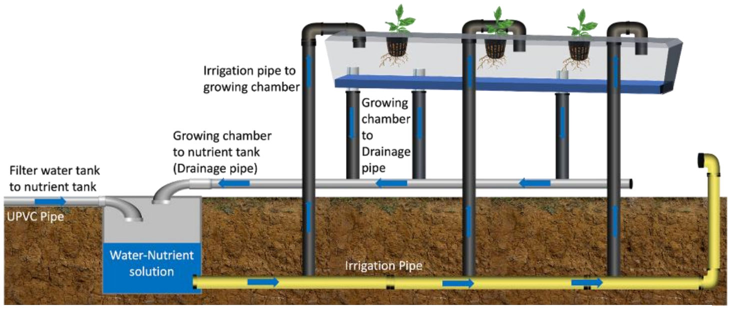

Figure 2: Growing chamber for soil-less farming for advanced agriculture (Ack: Eeki automation pvt ltd.).

Keyword: Polymers

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Understanding Mucin-Albumin assembly using microrheology

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Mucus is a viscoelastic layer, which is found along the lining of various organs such as the eyes, nose, mouth and the entire GI tract. The function of the mucus layer differs with its location in the body. For example, in the intestines, it protects the epithelial cell layers from the pathogens and creates a microenvironment which balances the normal gut microflora thereby facilitating a symbiotic relationship. Alteration of the rheology of the mucus layer leads to various disease conditions such as cystic fibrosis, Crohn's disease, and gastric ulcers, among others. Mucus consists of various mucins along with proteins such as immunoglobulin, lysozyme, and albumin. In the present study[1], we explore the effect of pH on the interactions between bovine serum albumin (BSA) and porcine gastric mucins using diffusing wave spectroscopy (DWS). The study shows that BSA actively binds with mucin to form mucin–BSA complexes, which is largely driven by electrostatic interactions.

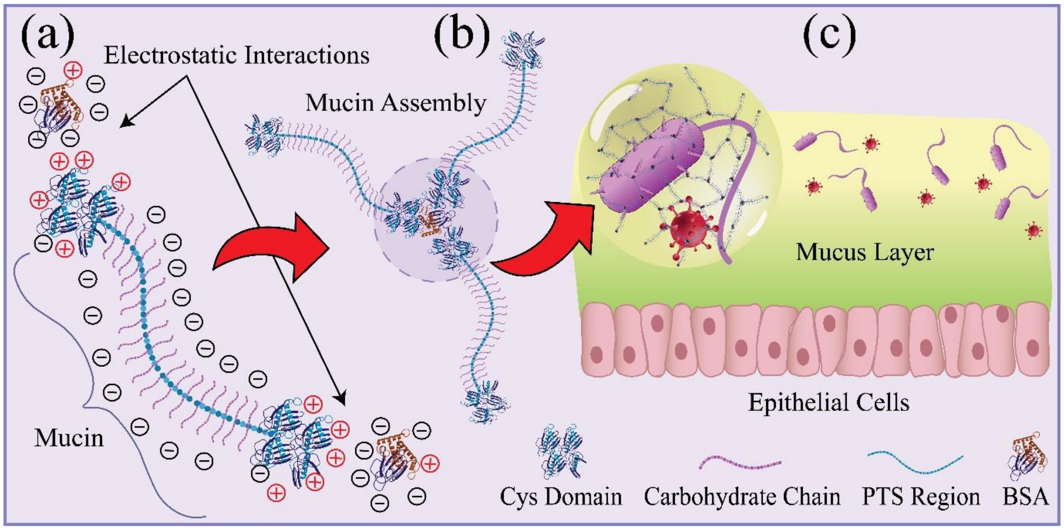

Figure 1: Caption of the Figure.

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Ultra-sensitive Protein Detection at the Aqueous-Liquid Crystal Droplet Interface using Microfluidic Engineering and Acoustic Patterning

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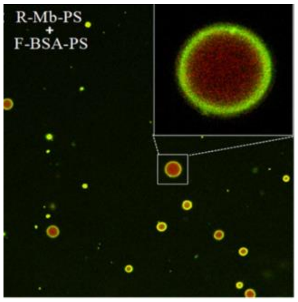
Liquid crystals (LC) have recently attracted considerable attention for sensing applications. Sensing using LCs is based on the changes in their topological defects giving rise to different optical textures, that can be viewed user a polarized light microscope. For biosensing, LC molecules should be sensitive towards proteins. However, polarity mismatch between proteins and LC molecules inhibits favorable interactions that can allow any sensing. In the talk I will describe a facile method for bridging such a miscibility gap between proteins and LC molecules. Protein-sequestered LC emulsion droplets based on the uptake of surface-engineered protein-polymer surfactant core-shell bioconjugates, will be demonstrated. Further, we will show that differences in the uptake behaviour can allow spontaneous positional assembly of multiple proteins in the LC droplets. Applications can be envisaged by the use of spatially separated glucose oxidase and horse radish peroxidase enzymes to produce LC droplets capable of housing an enzyme cascade reaction. At the end, in a quest towards developing functioning devices, I will show the use of flow focusing-based microfluidic and acoustic trapping technologies for developing a label-free and generic method to detect proteins using 1-D or 2-D assemblies of UV-treated LC droplets. Our methodologies thus opens several pathways for the development of bioactive liquid crystal droplets and could have potential applications in the optical sensing of biomolecular substrates.



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Fabrication of block copolymer membrane: What can be learned from coarse-grained models?

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SNIPS refers to the combination of evaporation-induced self-assembly (EISA) and subsequent, nonsolvent-induced phase separation (NIPS) of block copolymer-solvent systems and provides a bottom-up approach to fabricate integral-asymmetric, isoporous block copolymer membranes.[1] Initially, EISA creates a self-assembled, well-ordered, functional top layer of perpendicular cylindrical domains.[2,3] Subsequently, as the film contacts the nonsolvent (coagulation bath), NIPS fabricates a macroporous mechanical support.[4] To optimize permeability, selectivity, longevity, and cost, and to rationally design fabrication processes, direct insights into the spatiotemporal structure evolution are necessary.

Using a single, coarse-grained, particle-based model in conjunction with an efficient, multi-GPU-implementation of the SCMF algorithm, we study both processes, EISA and NIPS, focusing on the complex interplay between evaporation and solvent-nonsolvent exchange, micro- and macrophase separation, and kinetic arrest as the plasticizing solvent leaves the dense, polymer-rich domains (see Figur 1 that presents the density of majority component of the block copolymer). The simulations[4] identify a process window that allows for the successful fabrication of integral-asymmetric, isoporous diblock copolymer membranes, and contribute to understanding the role of the different structural and thermodynamic (e.g., solvent selectivity for the block copolymer components) as well as kinetic (e.g., plasticizing effect of the solvent) characteristics.

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Using swelling of polymer thin films to investigate the tightly bound layer at a polymer/substrate interface

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Experimental evidence indicates that a polymer layer that is strongly adsorbed and therefore tightly bound to an attractive substrate can exist in supported polymer thin films and polymer nanocomposites [1]. Typically this tightly bound layer can be up to a few tens of nanometres thick and given its influence on the physical properties, in situ techniques that can shed light on its characteristics without unduly disturbing it are desirable. Recently, we introduced an approach to estimate the thickness of the tightly bound layer at a polymer/substrate interface using the swelling of polymer thin films when exposed to solvent vapour. The approach was tested using thin films of thickness several tens to several hundred nanometres of two hydrophilic polymers, chitosan [2] and poly(vinyl alcohol) (PVA) [3] spin coated onto prepared silicon wafers. For the two polymers, the time dependence of the thin film thickness during swelling was studied using spectroscopic ellipsometry. Assuming that the tightly bound layer cannot swell when exposed to solvent vapour, we found that a single time-dependent swelling ratio could describe the swelling of *all* of the thin films investigated. We also deduced that the tightly bound layer was approximately 18 nm for chitosan and 15 nm for PVA. To corroborate the aforementioned approach, the swelling of the PVA thin films was also investigated using X-ray reflectivity. Electron density profiles determined by modelling the X-ray reflectivity data clearly indicated that at the polymer/substrate interface there exists a polymer layer of a slightly higher density than the rest of the film. The thickness of this polymer layer was found to be approximately 15 nm, consistent with the thickness of the tightly bound layer determined from the spectroscopic ellipsometry measurements. If time permits, I will comment on the implications of the aforementioned findings for other systems where one can expect tightly bound polymer layers at the polymer/substrate interface to play a role.

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Enhanced efficiency of water desalination in nanostructured thin-film membranes with polymer grafted nanoparticles

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Polyamide composite membranes are the state-of-the-art ubiquitous platforms to desalinate water at scale. We have developed a novel, transformative platform where the performance of such membranes is significantly and controllably improved by depositing thin films of polymethylacrylate (PMA) grafted silica nanoparticles (PGNPs) through the Langmuir–Blodgett method. Our key practically important finding is that these constructs can have unprecedented selectivity values (i.e., ∼250–3000 bar^{-1}, > 99.0% salt rejection) at reduced feed water pressure while maintaining acceptable water permeance A (= 2–5 $\mathrm{L\ m^{-2}\ h^{-1}\ Bar^{-1}}$) with as little as 5–7 PGNP layers, N. Interestingly, while water permeance, A shows non-monotonic dependence with N and graft PMA molecular weight, M_n, salt permeance shows strong decrease with increasing M_n and N leading to the observed unprecedented desalination efficiency.

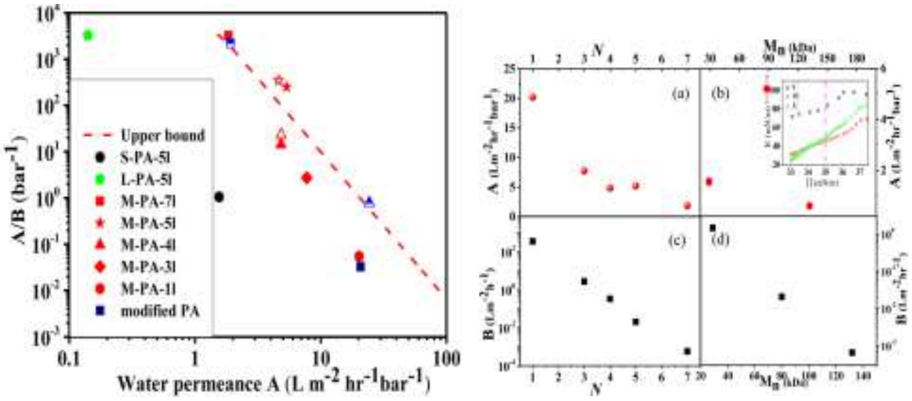

Figure 1: Left – Permselectivity **A/B** vs Water Permeance, **A** for various membranes. Right – Grafted Polymer molecular weight, M_n, and PGNP layer number, **N**, dependence of Water and salt permeance, **B**.

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Equilibration pathways beyond density fluctuations: the Slow Arrhenius Process

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The properties of an ensemble of objects at thermodynamic equilibrium do not change with time. Experience tells us, however, that such observation is rarely encountered in nature. The transformation of buds into flowers and then fruits, the rearrangements of plates on the surface of planets, and even the whole human body over its lifetime are just a few, among the many, examples of systems far from thermodynamic equilibrium.

At the molecular level, equilibration kinetics –the time evolution of a system's properties toward a less energetic state– are intimately coupled to molecular motion. In line with the Onsager's regression hypothesis [1], the macroscopic relaxation of a nonequilibrium system (dissipation) obeys the same laws of molecular dynamics in equilibrium conditions (spontaneous microscopic fluctuations).

In the case of liquids, equilibration is usually driven by the so-called a-modes, which are responsible for density fluctuations and require time scales quickly diverging upon cooling [2]. Growing experimental evidence indicates, however, the presence of a different, alternative pathway of weaker temperature dependence [3]. Such equilibration processes exhibit a temperature-invariant activation barrier, on the order of 100 kJ mol^{-1}. We have recently identified the underlying molecular process responsible for this class of Arrhenius equilibration mechanisms with a slow mode (SAP), universally observed in the liquid dynamics of thin films [4]. The SAP, which we show is intimately connected to high-temperature rheological behavior [5], can efficiently drive melts and glasses toward more stable, less energetic states. Based on the experimental findings collected so far on polymers and small molecules, we present a new framework for the equilibration of materials considering the contributions of both the SAP and the α–modes. In support of its potential, we demonstrate that our model is capable to provide quantitative predictions on the adsorption rate of polymers, a key parameter for the performance and durability of ultrathin polymer films.

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Peeling a thin sheet from a liquid surface

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The nature of peeling fronts, where a thin solid sheet is being detached from a bulk phase, has been an active research area since 1930, when Obreimoff studied the *discontinuity* of the film's curvature at the contact line with a bulk solid, and demonstrated the usefulness of the consequent contact condition for measuring solid surface energies. In this presentation, I will talk about the elasto-capillary version of this phenomenon, where a solid sheet peels off a bulk liquid phase. In this case, the stresses induced by capillary action play a key role and I will show that that the solid-fluid interfacial energies may affect the thermodynamic distribution of stresses within the solid body, but do not affect the mechanical response of the thin film to external forces. Further, the film's curvature remains continuous but its derivative exhibits a discontinuity, leading to a *cusp* in the curvature.

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Indian Society of Rheology

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Structure of adsorbed water present in thin films on mica surface: Effect of exposed ions

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The water vapor present in atmosphere adsorb on all solid surface making a thin layer depending upon the adsorption capacity of solid surface. Understanding this solid−water (vapor) interfacial systems is relevant for both industrial and academic scenarios for their presence in wide areas ranging from tribology to geochemistry. Using grand canonical Monte Carlo simulations, we have investigated the role of monovalent (Li^+, Na^+ , and K^+) and divalent (Mg^{2+} and Ca^{2+}) cations on the structure and adsorption behavior of water on mica surface. The water density adjacent to the surface exhibits (a) oscillations due to hydration of surface cations (interfacial layer), (b) followed by a thick liquid-like layer. The thickness of the interfacial layer is strongly dependent on the hydration shell size and hydration energy of surface ions. Water molecules immediately next to the surface (contact layers) adsorb on ditrigonal (hexagonal) cavities of mica surface and form an ordered structure. The Li^+ , Na^+ , Mg^{2+} , and Ca^{2+} surface ions are co-adsorbed with water molecules on the ditrigonal cavities due to their smaller hydration shell. Majority of water molecules in the second contact layer hydrate the surface ions and, together with the rest of the water molecules, form hydrogen bonds among themselves. The adsorption isotherm of water on all ion-exposed mica surface exhibits three regimes: (a) an initial rapid increase in water loading for relative vapor pressure (p/p_0) ≤ 0.2 due to hydration of surface ions; (b) followed by a linear increase between $p/p_0 = 0.2$ and 0.7, where the hydrogen bond formation between the water molecules of the interfacial layer occurs; and (c) exponential growth beyond $p/p_0 = 0.7$ due to thickening of the liquid-like layer. We found that ion hydration energy and size of hydration shell play a crucial role in their structure adjacent to mica surface. The detailed understanding obtained from this work will be useful in identifying the role of ions in cloud formation, nano-tribological studies, and activities of biological molecules and catalysis

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Indian Society of Rheology

Role of nanoparticle architecture and polymer-nanoparticle interface in unconventional flow of polystyrene thin films

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We have studied the dewetting of polystyrene (PS) thin films when nanoarchitectured CdSe tetrapods (CdSeTP) are incorporated within PS matrix. CdSeTP was synthesized in a one-pot synthesis method.[1] While dewetting, we observed an unconventional phenomenon whereby dewetting dynamics of PS thin-films increases as we incorporate CdSeTP within the PS matrix.[2] Previous studies have documented a noteworthy reduction in dewetting of polystyrene (PS) thin films upon incorporating spherical CdSe quantum dots (CdSeQD).[3] Hence, our observation indicates the significance of nanoparticle architecture in influencing the flow characteristics (viscosity) of thin films. Furthermore, as we incorporate CdSeTP of increasing size into the PS thin films, we observe a corresponding increase in the flow (viscosity) of the thin films as a function of CdSeTP size. This surprising phenomenon can be explained by a decrease in PS thin film viscosity coupled with decreasing modulus as a function of CdSeTP size. The enhancement in flow after incorporation of CdSeTP can be attributed to increase of effective PS-CdSeTP interface area resulting in the decrease in viscosity which in turn increases the flow of the PS thin films. The results also indicate towards the role of non-equilibrium polymer chain conformations and the role of nanoarchitecture in influencing the flow of the PS thin films.

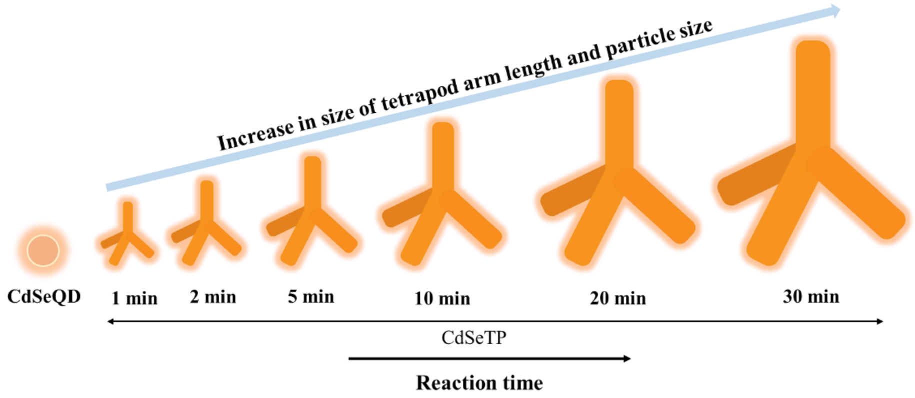

Figure 1: Schematic representation of growth of nanoparticles in a one-pot reaction.

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Rayleigh-Plateau Instability of a Viscoelastic Layer Coated on a Rigid Cylindrical Fibre

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Abstract

The Rayleigh-Plateau (RP) instability driven by surface tension is observed in day to day life such as water jet from a tap breaks up into droplets. Surface tension can play important role in soft solid materials like gels, elastomers and biological tissues. We study the RP instability of a viscoelastic solid layer coated on a rigid cylindrical fiber. We solve the governing equation for the deformation of soft solid and obtain the dispersion relation. We present the result of how the RP instability depends on elastocapillary length, the viscoelastic time scale, the rigid fiber radius and the substrate frictional coefficient.

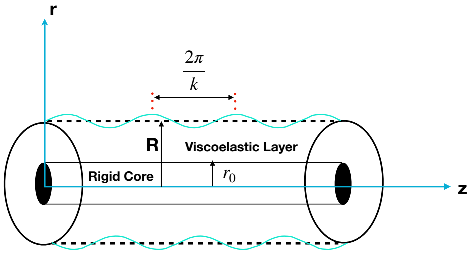

Figure 1: Schematic representation of soft viscous cylinder with rigid core.

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Effects of monomer sequence on the gas sorption and diffusion in a copolymer membrane

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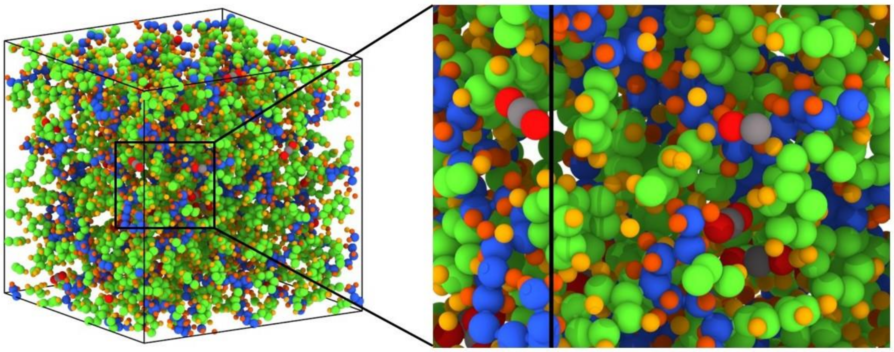
Abstract: Polymer membranes have gained significant attention in recent years due to their unique ability to selectively separate and transport gases and gas mixtures. These membranes consist of dense, compact polymer structures that can act as barriers for gas molecules, allowing for the separation of gases based on their size, shape, and chemical properties. Here, we employ molecular dynamics (MD) and grand canonical Monte Carlo (GCMC) simulations to investigate the influence of monomer sequence variations in a polystyrene (PS)-poly (methyl methacrylate) (PMMA) copolymer chain on the gas sorption and diffusion properties in the polymer melt [1]. The optimized potential for liquid simulation (OPLS) force field is utilized to model the polymer systems and Elementary Physical Model 2 (EPM2) for the CO_2 gas. We adopt an iterative procedure that combines MD simulations in the isothermal-isobaric ensemble (NPT) and the GCMC method to determine sorption isotherms and associated swelling effects. Further, we quantify diffusion coefficients for various gases from the long MD trajectories of gases in a polymer matrix. We demonstrate that the sequence of a copolymer can be an important design parameter for targeted gas separation applications [2]. The data provides new insights into the structure-property relationships of PS, PMMA, and their copolymers, highlighting the importance of monomer sequence in controlling the sorption and diffusion properties of polymeric materials.



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LIG coated Flexible and Reusable Textile based Dry Electrodes for Biopotential Sensing

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Abstract

Biopotential signals are used to assess organ function and and diagnose diseases. Biopotential electrodes are used to measure and record biopotentials by acting as an interface between biological tissue and electronic circuits. Wearable textile electrodes for biopotential sensing are a promising long-term health monitoring candidate. Smart textiles, which incorporate electronic elements directly into the fabric, provide a seamless way to incorporate sensors into clothing for a variety of applications. The direct writing of laser-induced graphene (LIG) on a Kevlar textile for the production of reusable dry electrodes for long-term ECG monitoring is described in this work. The electrode as-prepared has a high electrical conductivity and skin contact impedance of 100 ± 1 kΩ to 7.9 ± 2.7 kΩ for frequencies ranging from 40 Hz to 1 kHz, which is comparable to conventional Ag/AgCl wet electrodes. For clinical-quality performance, the results show comparable performance with significantly lower electrode-skin impedance. Even after several hours of use, these electrodes cause no skin irritation and work effectively without the need for skin preparation. Because of their flexibility and better match to the skin's modulus, the proposed dry electrodes are expected to provide greater comfort over time. The fabrication method is simple, cost-effective, and scalable, allowing for the production of arbitrary-shaped flexible electrodes for long-term biopotential monitoring.

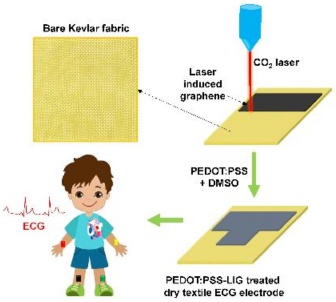

Figure : Schematic of LIG based dry electrode for biopotential (ECG) sensing.

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Smearing Technique For Liquid Viscosity Measurement

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Film coating, especially the blood smear coating are common techniques for generating thin films, or blood smears for monolayer analysis of the film. In such processes, a reservoir of the coating fluid is entrained between a substrate and a blade, where the blade is held at an angle above the substrate and is moved at a certain speed. The movement of the blade drags the entrained liquid thereby generating a thin film. We have built a simple device to cast a thin liquid film on to a glass slide with the aid of a moving blade held at an angle over the substrate (Fig. 1). The present work compares the film generation on a smear device with a model based on a Landau−Levich theory. The device operates at different constant speeds and based on the speed; one can generate desired films with a thickness gradient. We also show that the device has the capability of generating uniform thickness films by varying the operating speed. The model can also predict the viscosity of the film cast on the substrate by the measurement of the film length. Hence, the smearing device is effectively able to generate desired thickness films in addition to predicting viscosity. The device can hence find its application as a bed-side diagnostic tool in medical diagnostics and disease detection where a simple blood smear can be used in the estimation of the whole blood viscosity.

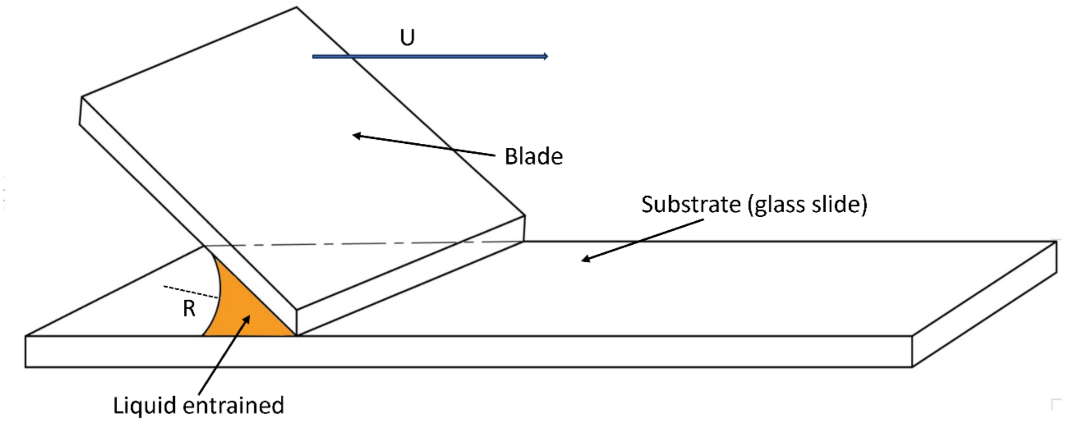

Figure 1: Smearing device schematic.

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Viscoelastic Bursting of Spin Coated Polymer Surfaces

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Preparation of polymer films often involves a transition of isolated polymers in a dilute solution to entangled glassy polymers [1]. Central to this transition is the rapid evaporation of solvent molecules, which may drag the macromolecules dissolved in the solution to the air-surface. Evaporation of small solvent molecules will be much faster than the enormously long time scales that polymers would take to self-diffuse [2]. This leads to the formation of a polymer rich skin layer, especially at the late stages of spin coating. Presence of such a dense polymeric layer at the surface necessitates a cooperative rearrangements of the chains at the surface for further evaporation of the solvent molecules trapped underneath [2,3]. At the same time, the Laplace pressure experienced by the solvent molecules progressively increases with the densification of the skin layer [4]. Here, we show such progressively increasing pressure results in a viscoelastic bursting of spin coated polymer films yielding porous surface structures. Beyond a critical thickness h_c, we observe such porous structures on films of different thickness (h) made using polymers of different molecular weight. We present one such example for polystyrene having molecular weight $M_w = 2000$ kg/mol in Fig.1. Interestingly, all different data (diameter (D_h) and depth of the holes (δ)) superposed when plotted as a function of the thickness (h_{tr}) of the thin film solution during the transition from the initial spin-off regime to evaporation dominated thinning of the solution [1].

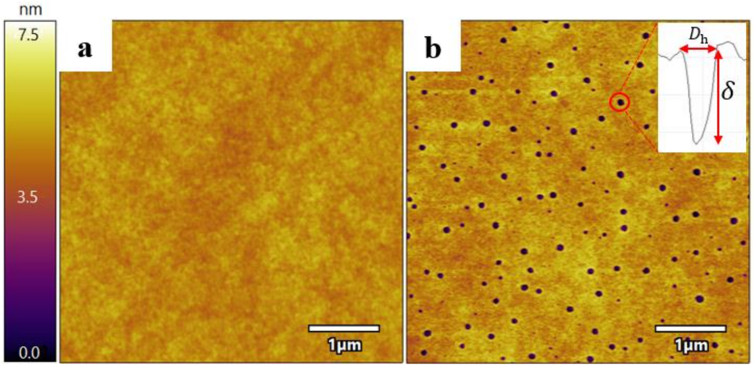

Figure 1: Surface morphology of spin-coated polymer films with thickness (a) $h \approx 25$ nm, and (b) $h \approx 180$ nm. Inset in (b) shows the height profile characterizing the definitions of depth (δ) and diameter (D_h) of the holes.

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Indian Society of Rheology

Charged diblock copolymer melts under shear: A molecular dynamics simulation study

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We study the behaviour of a thin film of charged diblock copolymer melts under mechanical shear using molecular dynamics simulation. A symmetric charged DBC melts forming vertically oriented lamellae is considered under transverse mode of shear. Above a critical shear rate, the vertically oriented lamellae undergo orientation transition. In this study, we investigate how the orientation transition, flow behaviour, chain deformation and counterion distribution depend on the shear rate. The macroscopic responses such as kinetic friction coefficient and shear viscosity are also studied.

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Linear stability analysis of a thin film of polar polymer solutions

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Ultrathin films of polymer solutions have a tendency to destabilize. In a typical thin film polymer solution, two distinct kinds of instabilities are observed, viz., de-wetting (long-wave) and decomposition (short-wave). De-wetting refers to the rupture of the continuous film to form isolated domains, while decomposition leads to phase separation within the polymer solution. The decomposition instability arises due to inter-molecular interactions between solute and solvent in the polymer solution. Thus, in a polar polymer solution, the dipole interactions significantly affect the stability of the film. This study mainly investigates the pattern of instabilities observed in a thin film of polar polymer solution. In order to model the system, the Flory-Huggins theory is employed to account for the non-polar interactions. For polar interactions, along with the Flory interaction parameter (χ_0), we incorporate an additional polar interaction parameter [1]. This parameter depends upon the concentration of the polymer (Φ) and the dipole moments of both polymer (μ_1) and solvent (μ_0). In a typical non-polar system, the decomposition mode remains dominant for a small range of concentrations. Our model predicts that this range is widened in the case of a polar polymer system. Also, the upper and lower limit of this range are directly affected by χ_0, μ_0 and μ_1. We also show that ignoring polar interactions can lead to incorrect predictions of the instability mode, including a complete loss of the decomposition mode. The long-wave de-wetting mode is not significantly affected by the polarity, because intermolecular interactions only affect the phase separation.

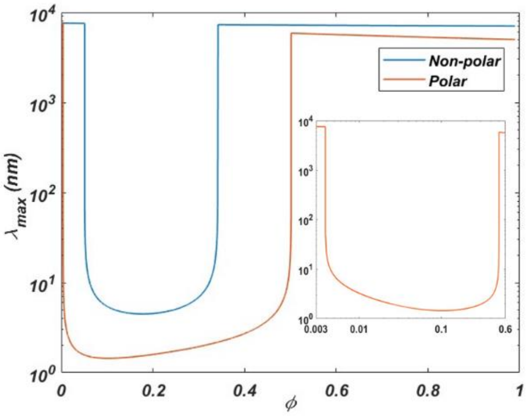

Figure 1: Wavelength (λ_{max}) corresponding to the maximum growth rate with polymer concentration (for both polar and non-polar cases). Decomposition mode (short wave) appears over a small range of concentrations with λ_{max} of the order $1nm$. The plot shows a wider range of concentrations for decomposition mode in the case of polar solution.

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Entropic and Enthalpic effect on interfacial jamming in polymer blend nanocomposite BIJELS

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Polymer nano-composites are interesting systems to study Bicontinuous interfacially jammed emulsion gels or BIJELs[1] both from a fundamental and application point of view. We have been studying the phase separation of PS-PVME bilayer which is an LCST binary system in presence of polymer(polystyrene) grafted gold nanoparticles with varying grafting density and chain length. It has been shown earlier from our group that it is possible to localize nanoparticles in a certain phase by tuning the grafted chain length of the PGNP [2]. When we raise the system above the LCST temperature, two processes occur simultaneously – the polymer binary undergoes phase separation via spinodal decomposition, and the nanoparticles relax in the viscoelastic polymer matrix. We have used in-situ X-ray photon correlation spectroscopy(XPCS)[3] to probe the nanoparticle dynamics at the interface during the phase separation above the LCST.

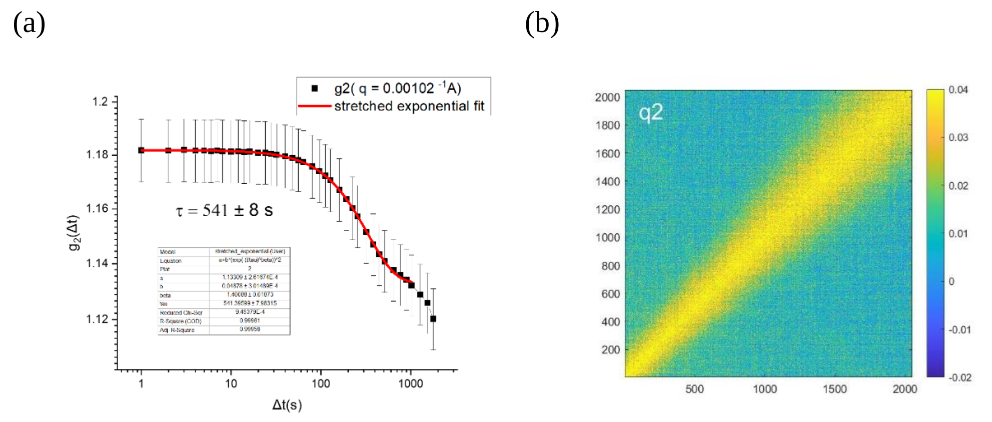

Fig. 1 : (a) Typical intensity-intensity autocorrelation function for bilayer PNC(PS+20Kd medium sigma PGNP at 120C, (b) Two-time correlation map showing non-equilibrium nature of the dynamics.

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Numerical study of instability of ferrofluid thin film using hybrid lattice Boltzmann method

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Ferrofluids are magnetizable liquids under the external magnetic field (H_o) due to the presence of magnetic nanoparticles. This numerical work studied the interfacial instability of ferrofluid thin film bounded by the non-magnetizable fluid (vapor) under magnetic field and van der Waals (vdW) interactions. Maxwell equations govern film dynamics along with the Navier-Stokes (NS) equations. Lattice Boltzmann method (LBM) is used to solve the NS equations, and Maxwell equations are solved by the finite volume method. An in-house hybrid lattice Boltzmann (HLBM) code is developed. The instability of the interface depends on the nature of vdW interactions, the direction of the external magnetic field, magnetic bond number $\left(Bo_m = \frac{\mu_o H_o^2 h_o}{2\gamma}\right)$, and permeability ratio$\left(\frac{\mu_l}{\mu_v}\right)$ of ferrofluid and bounding fluid. Under the repulsive vdW interactions $\left(A_{eff} < 0\right)$, the film completely wets the substrate. In this case, under the horizontal magnetic field observed traveling waves at the interface, whereas under the vertical magnetic field, undulations grow into peaks when $Bo_m > Bo_{cri}$. The number of peaks at the interface is a function of $Bo_m, d, \frac{\mu_l}{\mu_v}$, and the initial thickness of the film (h_o). And also, under the vertical magnetic field, observed pinching off the drop. At high values of Bo_m and $\frac{\mu_l}{\mu_v}$, elongation of the drop increases resulting in more than one daughter droplet, whereas at low values entire drop detaches from the substrate. Observed dewetting of the film under both the horizontal and vertical magnetic fields when $A_{eff} > 0$. The number of drops depends on the strength of the vdW interactions and magnetic force. Due to a decrease in adhesive force, observed entire drop detaching from the substrate.

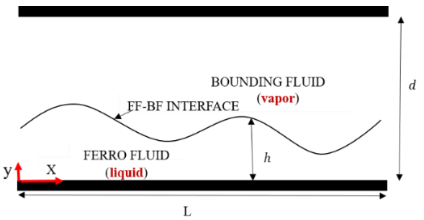

Figure 1: Schematic representation of the system

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Investigation of Bound Layers in Thin Films of Hydrophilic Polymers and Their Nanocomposites

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The conformation of polymer chains is strongly affected when in proximity to a solid, impenetrable surface. Depending on the interactions between the polymer and the surface, a distinct layer forms as chains become adsorbed onto the surface. Such a bound layer is known to significantly influence the structural and dynamic properties of overall polymer films and is well-documented [1]. In recent work, we introduced a novel approach for accurately determining the thickness and density of this bound layer. Our method relies on measuring the swelling kinetics of polymer films as they are exposed to solvent vapour [2,3]. In this study, we further investigate the properties of the bound layer within annealed thin films of a hydrophilic polymer, Poly(vinyl alcohol) (PVA), and its nanocomposites. The thickness of the bound layer, ds, was assessed using two independent techniques: analyzing the swelling kinetics [3] and applying Guiselin's approach [1]. The swelling kinetics of the films upon exposure to water vapour was measured using *in-situ* spectroscopic ellipsometry and X-ray reflectivity. The ds obtained using Guiselin's approach and the swelling measurements were consistent with each other and consistent with expectations, were essentially independent of the initial film thickness. Moreover, the physical properties of the bound layer, as observed in polymer nanocomposite films containing PVA and silica, will be presented.

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Banana leaf inspired anisotropic slippery surfaces

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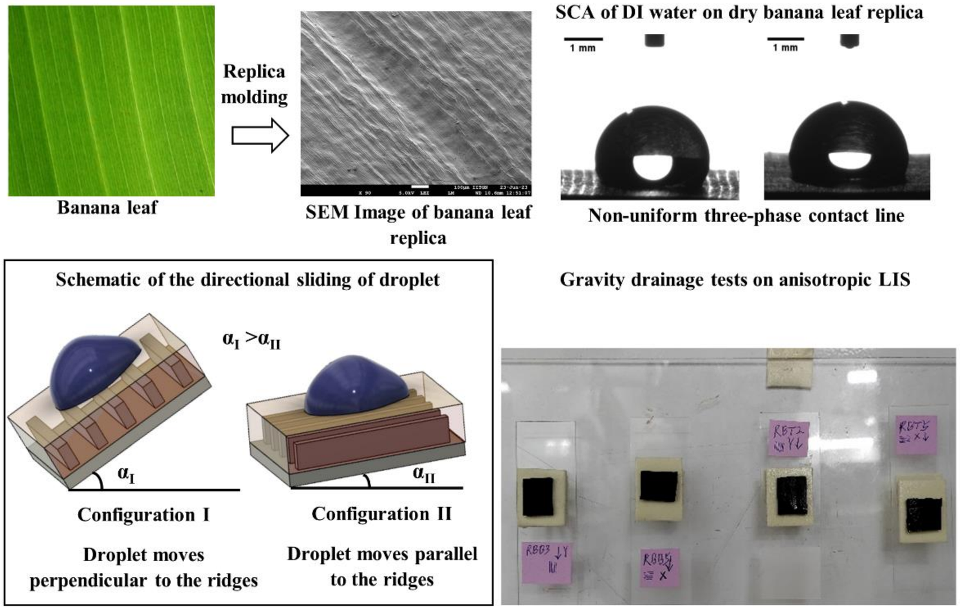
Slippery lubricant infused surfaces (LIS) with anisotropic micro features facilitate directional wettability that has a great potential in applications like water harvesting and bubble transport [1]. In this work, the anisotropic surface topography (parallel ridges) [2] of both top and bottom surfaces of natural banana leaves are replicated on silicone polymer via replica molding technique. The replicated textures from both the surfaces were characterized for Wenzel roughness with non-optical profilometry and scanning electron microscopy. Static contact angle measurements on the dry surfaces indicated non-uniformity of the three-phase contact line due to the anisotropic textures. Subsequently, the surfaces were coated with silicone oil with different film thicknesses ranging from 14 µm to 36 µm. Directional mobility of the droplet was observed by measuring the slide-off angles (SAs) on the lubricant coated surfaces for various film thicknesses. With decreasing film thickness the increase in SAs perpendicular to the ridges was more than the increase in SAs parallel to the ridges. At a certain film thickness the SA parallel to the ridges was lower than the SA perpendicular to the ridges for both the top and bottom surface replicas. Further gravity drainage tests suggested more drainage of lubricant along the ridge direction compared to the perpendicular to ridge direction. These observations indicate the effect of the anisotropic structures on the directional transportation of liquid as well as minimizing the lubricant depletion for anisotropic slippery surfaces.

Graphical abstract



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Effect of Plasticizer on Dewetting and Crazing Dynamics of Poly(p-tertbutylstyrene Thin Films

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We have studied crazing of long chain poly(p-tertbutylstyrene) (PtBS) under different constrains. Aging of pure PtBS films were done at temperatures close to and below glass transition temperature (Tg,*bulk*) of the polymer and quenched to room temperature. Scanning Electron Microscope (SEM) inspection for long chain polymers showed nanostructures within the crazes consisting of voids and fibrils, indicating craze. Rate of hole growth which further correlated with relaxation of preparation induced residual stresses (from spin-coating of thin PtBS films) was obtained by analysing optical micrographs taken with the help of microscope. Crazes appear throughout the film forming an interconnected network. A systematic study of craze propagation velocity, rate of hole growth, and fibril breaking time was done to understand the role of aging and residual stress in crazing of the film. While the craze propagation velocity increased with the duration of aging, indicating crazing stress localization and plastic deformation of the films; the dewetting studies showed a decrease in residual stress with increasing aging time. This contradiction raised the possibility of other stresses, such as thermal stress acting on the film or an increased elastic modulus resulting from possible re-entanglement of the chains during the crazing behavior.[1] Craze width and morphology of fibril structure were obtained from atomic force microscopy (AFM) micrographs. We have also added dioctyl phthalate (DOP) as a plasticizer and have observed opposing behaviour to that observed in pure PtBS. The effect plasticizer has on the flexibility and viscosity of the polymer becomes crucial in the formation of crazes. This differences in the crazing pattern and dynamics in pure PtBS and plasticized PtBS is further studied in detail.

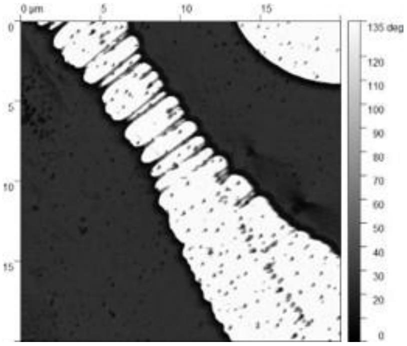

Figure 1: AFM micrograph of craze when aged for 24hrs and then quenched to room temperature (20µm x 20 µm image of a craze in a PtBS film (M_w = 1100 kD, thickness = 40 nm, aged at 120°C for 24hrs)

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Structure and water transport through block copolymers with a sulfonated hydrophilic block

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Block copolymers phase separate to form nanometer-scale morphologies and are attractive for membrane applications. In particular, block copolymers with a hydrophilic block afford water vapour transport and have potential for dehumidification. We investigate a pentablock ABCBA terpolymer comprising a central sulphonated polystyrene block, with hydrogenated isoprene (B) blocks for ductility and t-butyl styrene terminal (A) blocks for mechanical rigidity. The ionomeric midblock is hydrophilic and allows water vapour transport. We cast membranes from a toluene/propanol mixture that is a bad solvent for the midblock and from THF, that is a neutral solvent for all the blocks. We show that the water vapour transport rate (WVTR) is the same for membranes cast from these two solvent systems and is also independent of the membrane thickness. However, a change in the conditions under which the membrane is cast can decrease the WVTR by an order of magnitude. We probe the structure of these membranes using small angle X-ray scattering (SAXS) and correlate the WVTR with the membrane microstructure. Thus, we can relate the WVTR through a membrane with the structure formed on a nanometer scale.

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The effect of parametric forcing on the supercritical Marangoni instability

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This work focuses on the behavior of a liquid-passive fluid bilayer that is heated from the liquid side, in the absence of gravity, and subject to parametric forcing. Typically, such systems in the absence of parametric forcing exhibit Marangoni instability when the temperature difference exceeds a specific threshold value. This threshold varies with the perturbation wavenumber, according to a stability curve with two minima. The most unstable mode of the instability can be either long-wave or short-wave depending on the lateral confinement of the liquid layer. In the case of the long-wave mode, which is ordinarily observed in large confinements, experiments conducted by Vanhook et. al. [1] have shown the formation of dry spots.

This study aims to understand the effect of parametric forcing on the long-wave mode and investigate the mechanisms through which dry-out can be prevented by applying mechanical parametric forcing. This is achieved through linear stability analysis and computations using a nonlinear reduced-order model developed using the Weight Residual Integral Boundary Layer (WRIBL) technique. The results show that at low forcing frequencies, the liquid film can be rendered stable with a flat free surface within a certain range of forcing amplitudes, which decreases as the frequency increases. Outside this range, the flow becomes unstable, leading to the Marangoni instability and dry spot formation at lower forcing amplitudes, or Faraday instability accompanied by large free surface oscillations at higher forcing amplitudes. Beyond a critical value of the parametric frequency, stabilization to quiescent conditions cannot be achieved. Instead, we proceed directly from a Marangoni dominated flow characterized by long-wavelengths to a short-wavelength resonance-dominated flow, once again avoiding dry-out.

We show that two necessary prerequisites for the occurrence of a critical parametric frequency are the coexistence of Marangoni and Faraday instability modes and the finiteness of the container width.

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Effects of externally deposited nanoscale heterogeneities in thin polymer films on their interfacial behaviors

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Polymer nanocomposites have gained a considerable interest in polymer industry because of their capacity to enhance material performance and reliability. Consequently, over the last decade, scientists and engineers have exhibited a strong fascination to study the behavior of polymer nanocomposite materials. The macroscopic bulk mechanical behavior of a polymer primarily relies on its molecular weight and chemical composition [1]. In polymer nanocomposites, nanoparticles are induced externally via mixing or doping which act as external heterogeneities in the polymer matrix and subsequently affects the conformation and relaxation of polymer chains. As a result, these heterogeneities within polymers cause deviation in its local as well as bulk mechanical behavior from the equilibrium behavior. In this study we have investigated the role of external heterogeneities and their distribution on the bulk mechanical behavior of polymer matrix using standard mechanical measurements such as wrinkle formation, interfacial adhesion, and atomic force microscopy (AFM).

We have used silica (SiO_2) nanoparticles (20 nm) as external heterogeneity in the polymer polydimethylsiloxane (PDMS). We explored few techniques to obtain an optimum homogeneous dispersion of SiO_2 nanoparticles in bulk PDMS by adjusting the preparation parameters, using plasma-exposed SiO_2 nanoparticles. We observed that as the nanoparticle concentration in the polymer system increases, the interfacial adhesion, as well as the wavelength and amplitude of the wrinkle pattern, exhibit nonlinear changes [2]. During the measurements of local surface mechanical properties of PDMS-SiO_2 nanocomposite with the help of AFM, we observed the variation in the local elastic modulus and its correlation with the dispersion of nanoparticles within the polymeric system. These wrinkling phenomenon, interfacial adhesion and AFM measurements are connected with the macroscopic bulk mechanical behavior of the polymer, and also with the distribution and interaction of external nanoparticles with the system. The findings indicate that probing these heterogeneities could provide insight to understand the emergence of processing-induced deviations (internal heterogeneities) and the role of external impurities in the microscopic and macroscopic properties of polymers.

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