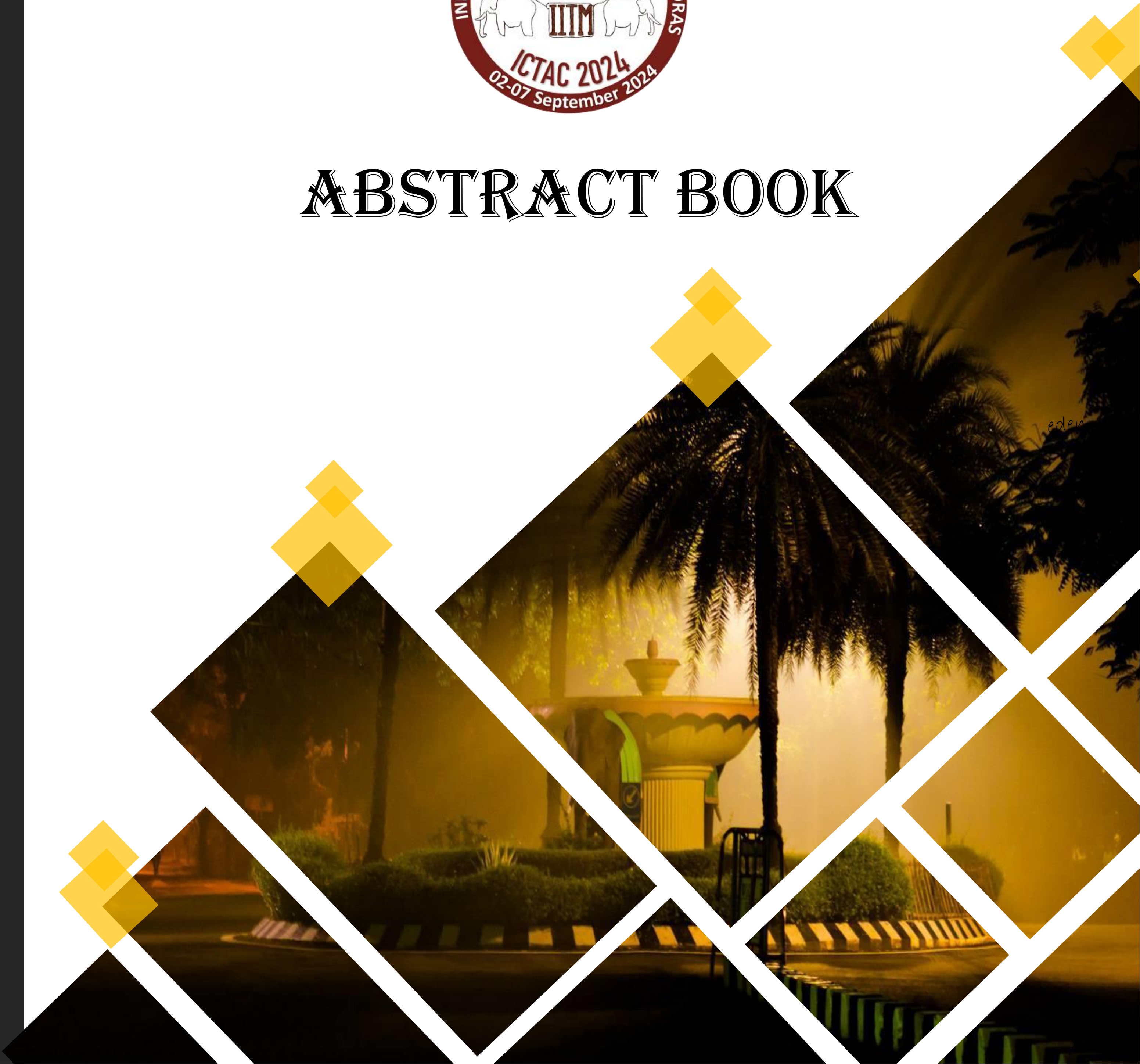
# 18th International Congress on Thermal Analysis and Calorimetry

# ICTAC 2024

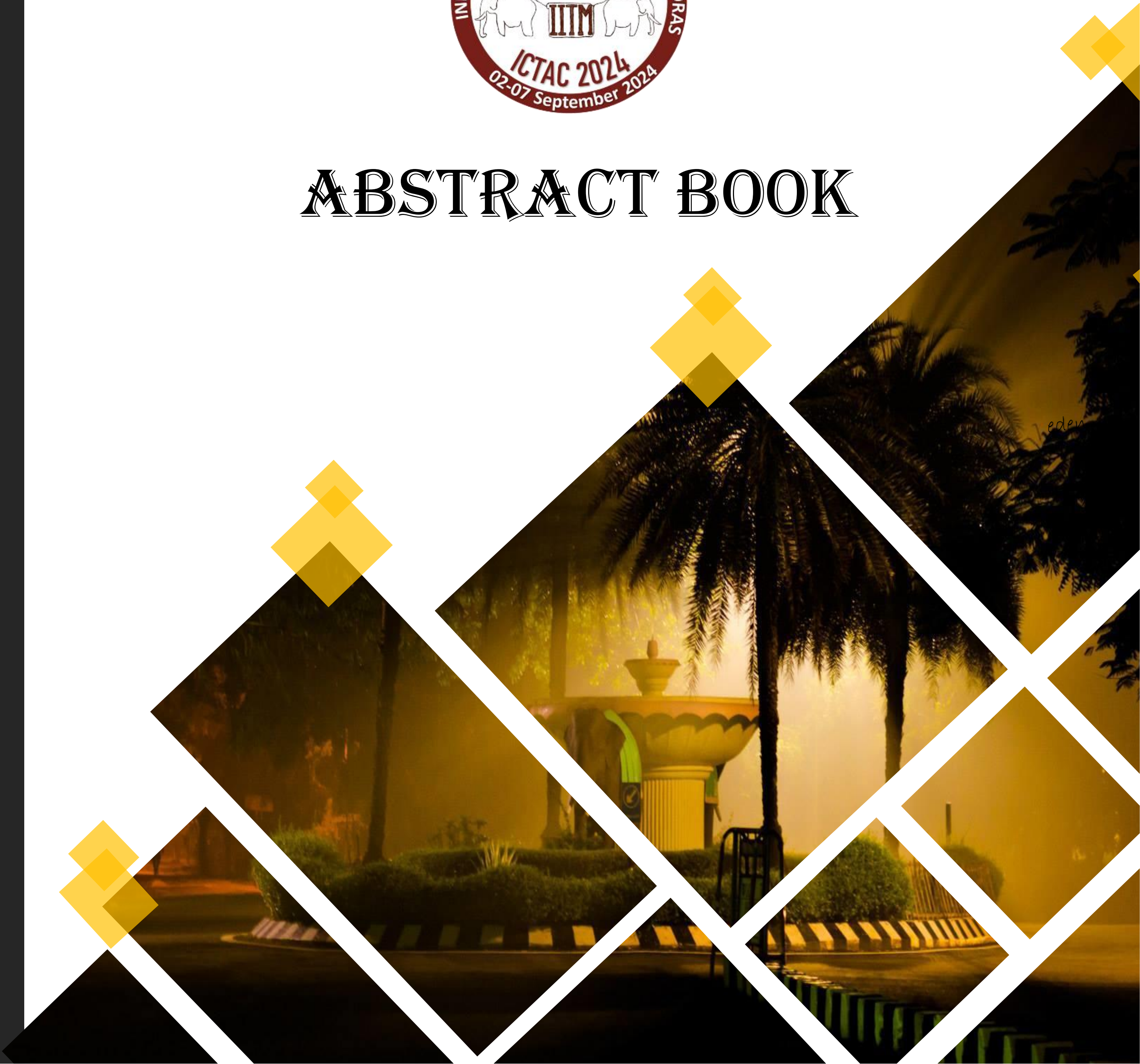
# ABSTRACT BOOK



# 18th International Congress on Thermal Analysis and Calorimetry

# ICTAC 2024

# ABSTRACT BOOK



**Indian Institute of Technology Madras**
**Chennai – 600 036**

Phone : 0091-44-2257 0694 / 0091-44-2257 8001
Fax : 0091-44-2257 8003 / 0091-44-2257 0509

**भारतीय प्रौद्योगिकी संस्थान मद्रास**
**चेन्नै – ६०० ०३६**

Email : kama@cse.iitm.ac.in / director@iitm.ac.in
Web : http://www.iitm.ac.in

**प्रो. वी. कामकोटि**
**Prof. V. Kamakoti**
**निदेशक**
**Director**

28th August 2024

# Message

It is with great pride and enthusiasm that we welcome you to the 18th International Congress on Thermal Analysis and Calorimetry (ICTAC 2024) and the 14th National Conference of the Indian Thermodynamics Society, hosted here at IIT Madras from September 2-7, 2024. This prestigious conference marks a historic moment as it is the first time ICTAC is being held in India.

At IIT Madras, we are honored to serve as the venue for this landmark event, which promises to be a convergence of cutting-edge research and collaborative spirit. The conference will spotlight diverse fields including material science, environmental science, and pharmaceutical research, bringing together over 400 distinguished scientists and researchers from across the globe.

ICTAC 2024 represents a significant opportunity for advancing scientific knowledge and fostering global collaborations in thermal analysis and calorimetry. We are excited to showcase our state-of-the-art research facilities and engage with international experts to explore new frontiers in our field.

We look forward to a successful and inspiring conference and to the new partnerships and discoveries that will emerge from this gathering.

V. Kamakoti

V. Kamakoti

डॉ जी सेकर
Dr. G. SEKAR
प्राध्यापक एवं विभागाध्यक्ष
Professor & Head

रसायन विज्ञान विभाग
Department of Chemistry
आई . आई . टी मद्रास / IIT Madras
चेन्नै/Chennai 600 036, भारत /India

Ph: 2257 4201/4200 /Fax: 2257 4202
Email: gsekar@zmail.iitm.ac.in; cyhead@zmail.iitm.ac.in

# Message

The Department of Chemistry at IIT Madras is delighted to host the 18th International Congress on Thermal Analysis and Calorimetry (ICTAC 2024) and the 14th National Conference of the Indian Thermodynamics Society. This event, taking place from September 2-7, 2024, is a testament to our commitment to advancing scientific research and fostering global academic partnerships.

Thermal analysis and calorimetry are pivotal in understanding material properties and processes across various scientific disciplines. This conference will cover a wide range of topics, including thermodynamics, kinetics, materials science, and environmental sciences. We anticipate a rich exchange of ideas and breakthroughs, driven by the participation of over 400 leading scientists and researchers from about 20 countries.

As the host department, we are excited to provide a platform for interdisciplinary dialogue and collaboration. The insights gained from this conference will not only enhance our academic pursuits but also contribute to addressing global challenges through innovative thermal analysis techniques.

We extend our warmest welcome to all delegates and look forward to a productive and engaging conference.

**Head, Department of Chemistry**
**IIT Madras**

**DEPARTMENT OF CHEMICAL ENGINEERING**
रासायनिक अभियांत्रिकी विभाग
**INDIAN INSTITUTE OF TECHNOLOGY MADRAS**
भारतीय प्रौद्योगिकी संस्थान मद्रास
**CHENNAI – 600 036, INDIA**
मद्रास चेन्नई-६०० ०३६ , भारत

**Dr. Niket S Kaisare**
Professor & HOD

Date: 27-07-2024

It is with great pleasure that the Department of Chemical Engineering at IIT Madras welcomes you to the 18th International Congress on Thermal Analysis and Calorimetry (ICTAC 2024) and the 14th National Conference of the Indian Thermodynamics Society. Scheduled from September 2 - 7, 2024, this conference represents a landmark event for both our institute and the global scientific community.

Thermal analysis and calorimetry are crucial for advancements in chemical engineering, influencing areas such as material synthesis, reaction kinetics, and process optimization. This conference will provide a unique opportunity to delve into these subjects, featuring presentations and discussions led by esteemed scientists and researchers from around the world.

We are proud to host this event, which aligns with our department's goals of fostering innovation and collaboration. ICTAC 2024 will serve as a platform for showcasing groundbreaking research, exploring new methodologies, and forging valuable international partnerships. We are eager to engage with our global peers and explore the transformative potential of thermal analysis in chemical engineering.

We extend a warm welcome to all participants and look forward to a conference filled with insightful discussions and productive collaborations.

**Head,**
**Department of Chemical Engineering,**
**IIT Madras**

**Phone:** 2257 4151 **Email:** chhead@iitm.ac.in **Website:** https://che.iitm.ac.in

# 18th International Congress on Thermal Analysis and Calorimetry (ICTAC 2024)

**02-07 September 2024, IIT Madras, India.**

☎ : +91-44-2257-5196 ✉ : ictac.iitm2024@gmail.com 🌐 : https://ge.iitm.ac.in/ICTAC-2024

Organizing committee
ICTAC 2024

## Welcome

Welcome to the 18th International Congress on Thermal Analysis and Calorimetry (ICTAC 2024) and the 14th National Conference of the Indian Thermodynamics Society! It is our great pleasure to host this prestigious event from September 2-7, 2024, at IIT Madras, India.

ICTAC 2024 marks a historic occasion as the first time this renowned conference is being held in India. This year's event will bring together over 400 delegates from about 20 countries, offering a vibrant forum for the latest advancements and discussions in thermal analysis and calorimetry.

Our conference will cover a broad spectrum of topics, including thermodynamics, kinetics, materials science, and environmental applications. We have curated a dynamic program featuring keynote speeches, thematic sessions, workshops and interactive discussions, aimed at fostering interdisciplinary collaborations and exploring new research frontiers.

We are excited about the opportunities ICTAC 2024 presents for scientific exchange and networking. Special sessions will focus on emerging research areas, and we anticipate engaging discussions that will drive future innovations in our field. Additionally, the conference will facilitate industry-academia interactions, poster presentations, and networking events to strengthen connections among researchers, students, and industry professionals.

We are grateful for the support of our esteemed international and national partners, including the International Confederation for Thermal Analysis and Calorimetry (ICTAC), Indian Thermodynamics Society (ITS), Amritsar, Indian Chemical Society (ICS), Kolkata, and Indian Council of Chemists (ICC), Agra. Their collaboration has been instrumental in bringing this conference to fruition.

We hope that your participation in ICTAC 2024 will be both enriching and inspiring. Thank you for joining us in making this conference a memorable and impactful event.

**Ramesh L. Gardas**
**IIT Madras**

**Jitendra S. Sangwai**
**IIT Madras**

**Ranjit Verma**
**Magadh University**

*in association with*

# Contents

# 18th International Congress on Thermal Analysis and Calorimetry (ICTAC 2024)

02-07 September 2024, IIT Madras, India

## Programme Schedule

| 1 Sept 2024 (Day: -1) | | | | | |
|---|---|---|---|---|---|
| **Time (IST)** | | **Hall - II** | | | |
| 15:30 | 18:30 | **ICTAC Executive committee meeting** | | | |

| 2 Sept 2024 (Day: 0) | | | | | |
|---|---|---|---|---|---|
| **Time (IST)** | | **Hall - II** | **Hall - IV** | | |
| 9:00 | 12:00 | **ICTAC Council meeting** | | | |
| **12:00** | **13:00** | **Registration** | | | |
| **13:00** | **13:45** | **Lunch Break** | | | |
| | | **Session 1** | | | |
| 13:45 | 14:15 | SATAC IL 01<br>**N B Singh** | **ESTAC Council meeting** | | |
| 14:15 | 14:45 | SATAC IL 02<br>**Namdeo Gajbhiye** | | | |
| 14:45 | 15:15 | SATAC IL 03<br>**Arun Pratap** | | | |
| 15:15 | 15:45 | SATAC IL 04<br>**Ranjit Verma** | | | |
| 15:45 | 16:15 | SATAC IL 05<br>**Ramesh L Gardas** | | | |
| 16:15 | 16:45 | SATAC IL 06<br>**Jitendra Sangwai** | | | |
| 16:45 | 17:00 | **Concluding Remarks** | | | |

| 3 Sept 2024 (Day: 1) | | | | | |
|---|---|---|---|---|---|
| **Time (IST)** | | **Main Auditorium** | **Hall - I** | **Hall - II** | **Hall - III** |
| 8:00 | 9:00 | **Registration** | | | |
| 9:00 | 10:15 | **Inauguration** | | | |
| **10:15** | **10:30** | **Tea Break** | | | |
| 10:30 | 11:30 | **Session 1A**<br>Robert Mackenzie Award lecture<br>**Jiri Malek** | | | |
| 11:30 | 12:20 | TA instrument ICTAC Award<br>**Chi-Min Shu** | | | |
| 12:20 | 13:05 | PL – 01<br>**Peter Šimon** | | | |
| **13:05** | **13:45** | **Lunch Break** | | | |

|  |  |  |  |  |  |
|---|---|---|---|---|---|
| 13:45 | 13:50 | **Session 2A** | **Session 1B** | **Session 1C** | **Session 1D** |
| 13:50 | 13:55 | PL - 01 (Track 1)<br>**Nand Kishore** | OP - 1 (Track 4)<br>YO | OP - 1 (Track 6)<br>SO | OP - 1 (Track 2)<br>SO |
| 13:55 | 14:00 |  |  |  |  |
| 14:00 | 14:05 |  | OP - 2 (Track 4)<br>YO |  |  |
| 14:05 | 14:10 |  |  | OP - 2 (Track 6)<br>YO | OP - 2 (Track 2)<br>SO |
| 14:10 | 14:15 |  |  |  |  |
| 14:15 | 14:20 | ITS AL – 01<br>**Dharmendra Singh** | OP - 3 (Track 4)<br>YO |  |  |
| 14:20 | 14:25 |  |  | OP - 3 (Track 6)<br>YO |  |
| 14:25 | 14:30 |  |  |  | OP - 3 (Track 2)<br>YO |
| 14:30 | 14:35 |  | OP - 4 (Track 4)<br>YO |  |  |
| 14:35 | 14:40 |  |  | OP - 4 (Track 6)<br>YO |  |
| 14:40 | 14:45 |  |  |  | OP - 4 (Track 2)<br>YO |
| 14:45 | 14:50 | ITS AL – 02<br>**Jyoti Rathee** | OP - 5 (Track 4)<br>YO |  |  |
| 14:50 | 14:55 |  |  | OP- 58 (Track 1)<br>YO |  |
| 14:55 | 15:00 |  |  |  | **Session 2D** |
| 15:00 | 15:05 |  | OP - 6 (Track 4)<br>YO |  | OP - 1 (Track 1)<br>SO |
| 15:05 | 15:10 |  |  | **Session 2C** |  |
| 15:10 | 15:15 |  |  | OP - 1 (Track 3)<br>SO |  |
| 15:15 | 15:20 | **Session 3A** | OP - 7 (Track 4)<br>YO |  | OP - 2 (Track 1)<br>SO |
| 15:20 | 15:25 | ITS AL – 03<br>**Vasim R Shaikh** |  |  |  |
| 15:25 | 15:30 |  |  | OP - 2 (Track 3)<br>YO |  |
| 15:30 | 15:35 |  | **Session 2B** |  |  |
| 15:35 | 15:40 |  | OP - 1 (Track 5)<br>SO |  | OP - 3 (Track 1)<br>SO |
| 15:40 | 15:45 |  |  | OP - 3 (Track 3)<br>YO |  |
| 15:45 | 15:50 | ITS AL – 04<br>**T Vasantha** |  |  |  |
| 15:50 | 15:55 |  | OP - 2 (Track 5)<br>YO |  |  |
| 15:55 | 16:00 |  |  | OP - 4 (Track 3)<br>YO | OP - 4 (Track 1)<br>YO |
| 16:00 | 16:05 |  |  |  |  |
| 16:05 | 16:10 |  | OP - 3 (Track 5)<br>YO |  |  |
| 16:10 | 16:15 |  |  | OP - 5 (Track 3)<br>SO | OP - 5 (Track 1)<br>YO |
| 16:15 | 16:20 | IL - 44 (Track 10)<br>SIL<br>**Sinjan Choudhary** |  |  |  |
| 16:20 | 16:25 |  | OP - 4 (Track 5)<br>YO |  |  |
| 16:25 | 16:30 |  |  |  |  |
| 16:30 | 16:35 |  |  |  |  |
| **16:35** | **16:45** | **Extended Tea Break** |  |  |  |
| **16:45** | **17:30** | **Poster Presentations (Track 1, Track 6, Track 8, Track 10)** |  |  |  |
| 17:30 | 17:35 | **Session 4A** |  | **ITS EC meeting and General Body Meeting** | **ICTAC General Assembly** |
| 17:35 | 17:40 | Industry slot – 01 |  |  |  |
| 17:40 | 17:45 |  |  |  |  |
| 17:45 | 17:50 |  |  |  |  |
| 17:50 | 17:55 | Industry slot - 02 |  |  |  |
| 17:55 | 18:00 |  |  |  |  |
| 18:00 | 18:05 |  |  |  |  |
| 18:05 | 18:10 |  |  |  |  |
| 18:10 | 18:15 | Industry slot - 03 |  |  |  |
| 18:15 | 18:20 |  |  |  |  |
| 18:20 | 18:25 |  |  |  |  |
| 18:25 | 18:30 |  |  |  |  |

| | | | | | |
|---|---|---|---|---|---|
| 18:30 | 19:15 | **Workshop of the ICTAC Thermodynamics &Thermochemistry committee** | | | **Workshop of the ICTAC Kinetics committee** |
| **19:15 onwards** | | **Cultural Program and Dinner (OAT - Open Air Theatre, IIT Madras)** | | | |

| **4 Sept 2024 (Day: 2)** | | | | | |
|---|---|---|---|---|---|
| **Time (IST)** | | **Main Auditorium** | **Hall - I** | **Hall - II** | **Hall - III** |
| 9:00 | 9:45 | **Session 5A**<br>PL – 02<br>**Andrei Rotaru** | | | |
| 9:45 | 10:30 | PL – 03<br>**Stefano Vecchio Ciprioti** | | | |
| 10:30 | 11:00 | Rigaku-ICTAC Young Scientist Award<br>**Jipeng Luo** | | | |
| **11:00** | **11:15** | **Tea Break** | | | |
| 11:15 | 11:20 | **Session 6A** | **Session 3B** | **Session 3C** | **Session 3D** |
| 11:20 | 11:25 | ICTAC Promising Researcher Award<br>**Birgit Mets** | OP - 1 (Track 7)<br>SO | OP - 1 (Track 8)<br>YO | OP - 6 (Track 1)<br>SO |
| 11:25 | 11:30 | | | | |
| 11:30 | 11:35 | | | OP - 2 (Track 8)<br>YO | |
| 11:35 | 11:40 | | OP - 2 (Track 7)<br>YO | | OP - 7 (Track 1)<br>SO |
| 11:40 | 11:45 | | | | |
| 11:45 | 11:50 | ICTAC TG AL – 01<br>**Tadas Dambrauskas** | | OP - 3 (Track 8)<br>YO | |
| 11:50 | 11:55 | | OP - 3 (Track 7)<br>YO | | |
| 11:55 | 12:00 | | | | OP - 8 (Track 1)<br>SO |
| 12:00 | 12:05 | ICTAC TG AL – 02<br>**Kylian Hallavant** | | OP - 5 (Track 5)<br>YO | |
| 12:05 | 12:10 | | OP - 4 (Track 7)<br>YO | | |
| 12:10 | 12:15 | | | | |
| 12:15 | 12:20 | ICTAC TG AL – 03<br>**Mito Hotta** | | OP - 6 (Track 5)<br>YO | OP - 9 (Track 1)<br>YO |
| 12:20 | 12:25 | | OP - 5 (Track 7)<br>YO | | |
| 12:25 | 12:30 | | | | |
| 12:30 | 12:35 | ICTAC TG AL – 04<br>**Francesca Saitta** | | OP - 7 (Track 5<br>YO | |
| 12:35 | 12:40 | | OP - 6 (Track 7)<br>YO | | OP - 10(Track 1)<br>YO |
| 12:40 | 12:45 | | | | |
| 12:45 | 12:50 | | | | |
| **12:50** | **13:45** | **Lunch Break** | | | |

| 13:45 | 13:50 | Session 7A | Session 4B | Session 4C | Session 4D |
|---|---|---|---|---|---|
| 13:50 | 13:55 | IL - 02 (Track 1)<br>**Sohel Murshed** | OP - 8 (Track 4)<br>YO | IL - 03 (Track 1) SIL<br>**Ajaya Battarai** | IL - 27 (Track 5)<br>**Kinga Pielichowska** |
| 13:55 | 14:00 | | | | |
| 14:00 | 14:05 | | OP - 9 (Track 4)<br>YO | | |
| 14:05 | 14:10 | | | OP - 11 (Track 1)<br>YO | |
| 14:10 | 14:15 | | | | |
| 14:15 | 14:20 | IL - 45 (Track 10)<br>**Arvind Kumar** | OP - 10 (Track 4)<br>YO | | IL - 28 (Track 5)<br>**Debashis Chakraborty** |
| 14:20 | 14:25 | | | OP - 12 (Track 1)<br>YO | |
| 14:25 | 14:30 | | | | |
| 14:30 | 14:35 | | OP - 11 (Track 4)<br>YO | | |
| 14:35 | 14:40 | | | OP - 13 (Track 1)<br>YO | |
| 14:40 | 14:45 | | | | |
| 14:45 | 14:50 | IL - 46 (Track 10)<br>**Homendra Naorem** | OP - 12 (Track 4)<br>YO | | IL - 29 (Track 5) SIL<br>**Hema Chandra Kotamarthi** |
| 14:50 | 14:55 | | | OP - 14 (Track 1)<br>YO | |
| 14:55 | 15:00 | | | | |
| 15:00 | 15:05 | | OP - 13 (Track 4)<br>YO | | |
| 15:05 | 15:10 | | | OP - 15 (Track 1)<br>YO | IL - 30 (Track 5) SIL<br>**Jayaramulu Kolleboyina** |
| 15:10 | 15:15 | | | | |
| 15:15 | 15:20 | IL - 47 (Track 10)<br>**Sudhakar Dhondge** | OP - 14 (Track 4)<br>YO | | |
| 15:20 | 15:25 | | | OP - 16 (Track 1)<br>YO | |
| 15:25 | 15:30 | | | | IL - 31 (Track 5) SIL<br>**Yamini Sudha Sistla** |
| 15:30 | 15:35 | | OP - 15 (Track 4)<br>YO | | |
| 15:35 | 15:40 | | | OP - 17 (Track 1)<br>YO | |
| 15:40 | 15:45 | | | | |
| 15:45 | 15:50 | IL - 48 (Track 10)<br>**Tamal Banerjee** | OP - 16 (Track 4)<br>YO | | Industry slot - 04 |
| 15:50 | 15:55 | | | OP - 18 (Track 1)<br>YO | |
| 15:55 | 16:00 | | | | |
| 16:00 | 16:05 | | OP - 17 (Track 4)<br>YO | | |
| 16:05 | 16:10 | | | | |
| 16:10 | 16:15 | | | | |
| **16:15** | **16:30** | **Extended Tea Break** | | | |
| **16:30** | **17:15** | **Poster Presentation (Track 2, Track 3, Track 4, Track 5, Track 7)** | | | |
| 17:15 | 17:20 | Session 8A | Session 5B | Session 5C | **Workshop of the ICTAC Standards and Nomenclature committee** |
| 17:20 | 17:25 | IL - 37 (Track 8)<br>**Dimitrios Bikiaris** | OP - 5 (Track 2)<br>SO | OP - 19 (Track 1)<br>YO | |
| 17:25 | 17:30 | | | | |
| 17:30 | 17:35 | | | OP - 20 (Track 1)<br>YO | |
| 17:35 | 17:40 | | OP - 6 (Track 2)<br>YO | | |
| 17:40 | 17:45 | | | | |
| 17:45 | 17:50 | IL - 38 (Track 8)<br>SIL<br>**Deepak Kumar Ojha** | | OP - 21 (Track 1)<br>YO | |
| 17:50 | 17:55 | | OP - 7 (Track 2)<br>YO | | |
| 17:55 | 18:00 | | | | |
| 18:00 | 18:05 | | | OP - 22 (Track 1)<br>YO | |
| 18:05 | 18:10 | IL - 51 (Track 10)<br>SIL<br>**Sushma Ijardar** | OP - 8 (Track 2)<br>YO | | |
| 18:10 | 18:15 | | | | |
| 18:15 | 18:20 | | | OP - 23 (Track 1)<br>YO | |
| 18:20 | 18:25 | | | | |
| 18:25 | 18:30 | | | | |
| **19:15 onwards** | | **Dinner** | | | |

| **5 Sept 2024 (Day: 3)** | | | | | |
|---|---|---|---|---|---|
| **Time (IST)** | | **Main Auditorium** | **Hall - I** | **Hall - II** | **Hall - III** |
| 9:15 | 9:45 | **Session 9A**<br>IL - 04 (Track 1)<br>**Zhiwu Yu** | | | |
| 9:45 | 9:50 | IL - 05 (Track 1)<br>**Alfréd Kállay-Menyhárd** | **Session 6B** | **Session 6C** | **Session 5D** |
| 9:50 | 9:55 | | OP - 09 (Track 2)<br>YO | OP - 24 (Track 1)<br>YO | IL - 07 (Track 1)<br>**Amalendu Pal** |
| 9:55 | 10:00 | | | | |
| 10:00 | 10:05 | | OP - 10 (Track 2)<br>YO | OP - 25 (Track 1)<br>YO | |
| 10:05 | 10:10 | | | | |
| 10:10 | 10:15 | | | | |
| 10:15 | 10:20 | IL - 06 (Track 1)<br>**Vilko Mandić** | OP - 11 (Track 2)<br>YO | OP - 26 (Track 1)<br>YO | IL - 08 (Track 1)<br>**Dilip Dagade** |
| 10:20 | 10:25 | | | | |
| 10:25 | 10:30 | | | | |
| 10:30 | 10:35 | | OP - 12 (Track 2)<br>YO | OP - 27 (Track 1)<br>YO | |
| 10:35 | 10:40 | | | | |
| 10:40 | 10:45 | | | | |
| **10:45** | **11:00** | **Tea Break** | | | |
| 11:00 | 11:05 | **Session 10A** | **Session 7B** | **Session 7C** | **Session 6D** |
| 11:05 | 11:10 | IL - 49 (Track 10)<br>SIL<br>**Md. Sayem Alam** | OP - 13 (Track 2)<br>YO | OP - 28 (Track 1)<br>YO | IL - 09 (Track 1)<br>**Amiya Panda** |
| 11:10 | 11:15 | | | | |
| 11:15 | 11:20 | | OP - 14 (Track 2)<br>YO | OP - 29 (Track 1)<br>YO | |
| 11:20 | 11:25 | IL - 50 (Track 10)<br>SIL<br>**Sangesh Zodape** | | | |
| 11:25 | 11:30 | | | | |
| 11:30 | 11:35 | | OP - 15 (Track 2)<br>YO | OP - 30 (Track 1)<br>YO | IL - 55 (Track 10)<br>**Ranjan Dey** |
| 11:35 | 11:40 | | | | |
| 11:40 | 11:45 | IL - 52 (Track 10)<br>SIL<br>**Vickramjeet Singh** | | | |
| 11:45 | 11:50 | | OP - 16 (Track 2)<br>YO | OP - 31 (Track 1)<br>YO | |
| 11:50 | 11:55 | | | | |
| 11:55 | 12:00 | | | | |
| 12:00 | 12:05 | IL - 53 (Track 10)<br>SIL<br>**Ashwani Kumar Sood** | OP - 17 (Track 2)<br>YO | OP - 32 (Track 1)<br>YO | OP - 01 (Track 10)<br>YO |
| 12:05 | 12:10 | | | | |
| 12:10 | 12:15 | | | | |
| 12:15 | 12:20 | | OP - 18 (Track 2)<br>YO | OP - 33 (Track 1)<br>YO | OP - 02 (Track 10)<br>YO |
| 12:20 | 12:25 | IL - 54 (Track 10)<br>SIL<br>**Poonam Patyar** | | | |
| 12:25 | 12:30 | | | | |
| 12:30 | 12:35 | | OP - 19 (Track 2)<br>YO | OP - 34 (Track 1)<br>YO | OP - 03 (Track 10)<br>YO |
| 12:35 | 12:40 | | | | |
| 12:40 | 12:45 | IL - 39 (Track 8)<br>SIL<br>**Meena Bisht** | | | |
| 12:45 | 12:50 | | OP - 20 (Track 2)<br>YO | OP - 35 (Track 1)<br>YO | OP - 04 (Track 10)<br>YO |
| 12:50 | 12:55 | | | | |
| 12:55 | 13:00 | | | | |
| **13:00** | **13:15** | **Best poster announcement at main auditorium** | | | |
| **13:15** | **13:45** | **Lunch Break** | | | |
| **13:45** | **19:00** | **Trip to Mahabalipuram** | | | |
| **19:15 onwards** | | **Dinner** | | | |

| **6 Sept 2024 (Day: 4)** | | | | | |
|---|---|---|---|---|---|
| **Time (IST)** | | **Main Auditorium** | **Hall - I** | **Hall - II** | **Hall - III** |
| 9:00 | 9:05 | **Session 11A** | **Session 8B** | **Session 8C** | **Session 7D** |
| 9:05 | 9:10 | IL - 10 (Track 1)<br>**Eswarmoorthy Muthusamy** | OP - 08 (Track 5)<br>YO | IL - 15 (Track 1)<br>**Riyazuddeen** | IL - 32 (Track 6)<br>**Sarma Pisupati** |
| 9:10 | 9:15 | | | | |
| 9:15 | 9:20 | | OP - 09 (Track 5)<br>YO | | |
| 9:20 | 9:25 | | | | |
| 9:25 | 9:30 | | | | |
| 9:30 | 9:35 | IL - 11 (track 1)<br>**Surianarayanan Mahadevan** | OP - 10 (Track 5)<br>YO | OP - 36 (Track 1)<br>SO | IL - 33 (Track 6) SIL<br>**Poonguzhali Elamvazhuthi** |
| 9:35 | 9:40 | | | | |
| 9:40 | 9:45 | | | | |
| 9:45 | 9:50 | | OP - 11 (Track 5)<br>YO | | |
| 9:50 | 9:55 | | | OP - 37 (Track 1)<br>YO | IL - 20 (Track 3)<br>**Kamalika Sen** |
| 9:55 | 10:00 | | | | |
| 10:00 | 10:05 | IL - 12 (Track 1) SIL<br>**M Hamsa Priya** | OP - 12 (Track 5)<br>YO | | |
| 10:05 | 10:10 | | | OP - 38 (Track 1)<br>YO | |
| 10:10 | 10:15 | | | | |
| 10:15 | 10:20 | | OP - 13 (Track 5)<br>YO | | |
| 10:20 | 10:25 | IL - 13 (Track 1) SIL<br>**Santosh Deosarkar** | | OP - 39 (Track 1)<br>YO | IL - 21 (Track 3)<br>**Sujata Mandal** |
| 10:25 | 10:30 | | | | |
| 10:30 | 10:35 | | OP - 14 (Track 5)<br>YO | | |
| 10:35 | 10:40 | | | OP - 40 (Track 1)<br>YO | |
| 10:40 | 10:45 | IL - 14 (Track 1) SIL<br>**Pardha Saradhi Maram** | | | |
| 10:45 | 10:50 | | OP - 15 (Track 5)<br>YO | | |
| 10:50 | 10:55 | | | OP - 41 (Track 1)<br>YO | |
| 10:55 | 11:00 | | | | |
| 11:00 | 11:05 | | | | |
| **11:05** | **11:15** | **Tea Break** | | | |
| 11:15 | 11:20 | **Workshop of the ICTAC Education committee** | **Session 9B** | **Session 9C** | **Session 8D** |
| 11:20 | 11:25 | | OP - 16 (Track 5)<br>YO | OP - 42 (Track 1)<br>YO | OP - 06 (Track 3)<br>SO |
| 11:25 | 11:30 | | | | |
| 11:30 | 11:35 | | OP - 17 (Track 5)<br>YO | OP - 43 (Track 1)<br>YO | |
| 11:35 | 11:40 | | | | OP - 07 (Track 3)<br>YO |
| 11:40 | 11:45 | | | | |
| 11:45 | 11:50 | | OP - 18 (Track 5)<br>YO | OP - 44 (Track 1)<br>YO | |
| 11:50 | 11:55 | | | | OP - 08 (Track 3)<br>YO |
| 11:55 | 12:00 | | | | |
| 12:00 | 12:05 | **Session 12A** | OP - 19 (Track 5)<br>YO | OP - 45 (Track 1)<br>YO | |
| 12:05 | 12:10 | IL - 42 (Track 9)<br>**Arun Tangirala** | | | OP - 09 (Track 3)<br>YO |
| 12:10 | 12:15 | | | | |
| 12:15 | 12:20 | | OP - 20 (Track 5)<br>YO | OP - 46 (Track 1)<br>YO | |
| 12:20 | 12:25 | | | | OP - 10 (Track 3)<br>YO |
| 12:25 | 12:30 | | | | |
| 12:30 | 12:35 | IL - 43 (Track 9)<br>**Edamana Prasad** | IL - 56<br>**Ranjit K Verma** | OP - 47 (Track 1)<br>YO | |
| 12:35 | 12:40 | | | | OP - 11 (Track 3)<br>YO |
| 12:40 | 12:45 | | | | |
| 12:45 | 12:50 | | | OP - 48 (Track 1)<br>YO | |
| 12:50 | 12:55 | | | | OP - 12 (Track 3)<br>YO |
| 12:55 | 13:00 | | | | |
| 13:00 | 13:05 | | | | |

| | | | | | |
|---|---|---|---|---|---|
| **13:05** | **13:40** | **Lunch Break** | | | |
| 13:40 | 13:45 | **Session 13A** | **Session 10B** | **Session 10C** | **Session 9D** |
| 13:45 | 13:50 | IL - 22 (Track 4)<br>**Pannuru Venkatesu** | OP - 4 (Track 8)<br>YO | OP - 49 (Track 1)<br>YO | IL - 34 (Track 7) SIL<br>**Sumit Bhawal** |
| 13:50 | 13:55 | | | | |
| 13:55 | 14:00 | | OP - 5 (Track 8)<br>YO | OP - 50 (Track 1)<br>YO | |
| 14:00 | 14:05 | | | | IL - 35 (Track 7) SIL<br>**Naved Malek** |
| 14:05 | 14:10 | | | | |
| 14:10 | 14:15 | IL - 23 (Track 4)<br>**Dip Saikia** | OP - 6 (Track 8)<br>YO | OP - 51 (Track 1)<br>YO | |
| 14:15 | 14:20 | | | | |
| 14:20 | 14:25 | | | | IL - 36 (Track 7) SIL<br>**Paurnima Talele** |
| 14:25 | 14:30 | | OP - 7 (Track 8)<br>YO | OP - 52 (Track 1)<br>YO | |
| 14:30 | 14:35 | | | | |
| 14:35 | 14:40 | | | | |
| 14:40 | 14:45 | IL - 24 (Track 4)<br>**Anima Nanda** | OP - 8 (Track 8)<br>YO | OP - 53 (Track 1)<br>YO | IL - 16 (Track 1)<br>**Rama Nand Rai** |
| 14:45 | 14:50 | | | | |
| 14:50 | 14:55 | | | | |
| 14:55 | 15:00 | | OP - 9 (Track 8)<br>YO | OP - 54 (Track 1)<br>YO | |
| 15:00 | 15:05 | | | | |
| 15:05 | 15:10 | | | | |
| 15:10 | 15:15 | IL - 25 (Track 4)<br>**Mahesh B** | OP - 10 (Track 8)<br>YO | OP - 55 (Track 1)<br>YO | IL - 18 (Track 2) SIL<br>**Kogularasu Sakthivel** |
| 15:15 | 15:20 | | | | |
| 15:20 | 15:25 | | | | |
| 15:25 | 15:30 | | OP - 11 (Track 8)<br>YO | OP - 56 (Track 1)<br>YO | |
| 15:30 | 15:35 | | | | IL - 40 (Track 8) SIL<br>**Gaurav Pandey** |
| 15:35 | 15:40 | | | | |
| 15:40 | 15:45 | Industry slot - 05 | OP - 12 (Track 8)<br>YO | OP - 57 (Track 1)<br>YO | |
| 15:45 | 15:50 | | | | |
| 15:50 | 15:55 | | | | |
| 15:55 | 16:00 | | | | |
| **16:00** | **16:15** | **Extended Tea Break** | | | |
| 16:15 | 16:20 | **Session 14A** | | | **Session 10D** |
| 16:20 | 16:25 | IL - 19 (Track 2)<br>**Kothandaraman Ramanujam** | | | IL - 41 (Track 8)<br>**Rajnish Kumar** |
| 16:25 | 16:30 | | | | |
| 16:30 | 16:35 | | | | |
| 16:35 | 16:40 | | | | |
| 16:40 | 16:45 | | | | |
| 16:45 | 16:50 | IL - 17 (Track 01)<br>**G. Venkatarathnam** | | | IL - 26 (Track 4)<br>**Sathyanarayana N. Gummadi** |
| 16:50 | 16:55 | | | | |
| 16:55 | 17:00 | | | | |
| 17:00 | 17:05 | | | | |
| 17:05 | 17:10 | | | | |
| 17:10 | 17:15 | | | | |
| **19:15 onwards** | | **Dinner** | | | |

| **7 Sept 2024 (Day: 5)** | | | | | |
|---|---|---|---|---|---|
| **Time (IST)** | | **Main Auditorium** | | | |
| 9:00 | 11:00 | **PANEL DISCUSSION AND VALEDICTORY** | | | |

| **Number** | **Name** | **Title of the presentation** |
|---|---|---|
| **PLENARY & AWARD LECTURES** | | |
| PL 01 | Peter Šimon | Methods based on the general rate equation – applications and limits |
| PL 02 | Andrei Rotaru | The generalized conversion functions for heterogeneous kinetics |
| PL 03 | Stefano Vecchio Ciprioti | Thermodynamic and Kinetic Perspectives to Monitor the Competition Between Decomposition and Vaporization in Ionic Liquids |
| PL 04 | Nand Kishore | Structure-Property-Energetics Relationships in Deriving Guidelines for Rational Drug Design: Thermodynamic Approach |
| RM Award | Jiri Malek | Universality of Master Plots in Thermal Analysis |
| TA-ICTAC Award | Chi-Min Shu | Critical safety challenges in Lithium-ion batteries: An examination thermal runaway and fire behaviors |
| Rigaku ICTAC Award | Jipeng Luo | Design and Construction of a Refrigerator-Cooled Adiabatic Calorimeter for Heat Capacity Measurement in Liquid Helium Temperature Region |
| ICTAC Promising Award | Birgit Mets | Thermal analysis and calorimetry as tools for assessing the properties of different oil shales and their conversion products |
| ITS AL 01 | Dharmendra Singh | Emerging prospective of role of solvents in biological process |
| ITS AL 02 | Jyoti Rathee | Unravelling Thermodynamics Signatures Accompanying Binding of Protein to Lipid Nanoparticles: A Spectroscopic and Calorimetric Analysis |
| ITS AL 03 | Vasim R Shaikh | Study of Molecular Interactions for the Supramolecules in Aqueous, Aqueous–Drug and Aqueous–KBr Solutions at 298.15 K |
| ITS AL 04 | T Vasantha | Thermodynamic Characterization of the Structural Basis for the Enhanced Solubility, Stability of Protein Model Compounds and Peptide Backbone Unit in Ammonium Based Ionic Liquids |
| ICTAC TG AL 01 | Tadas Dambrauskas | Calcium Silicate Hydrates with Intercalated Transition Metal Ions: Preparation Techniques, Thermal Properties, and Applications |
| ICTAC TG AL 02 | Kylian Hallavant | Influence of chemical composition and structure on the cooperative fluctuation in supercooled glass-forming liquids |
| ICTAC TG AL 03 | Mito Hotta | Thermal Dehydration Kinetics of Copper(II) Sulfate Pentahydrate across Different Water Vapor Pressures |
| ICTAC TG AL 04 | Francesca Saitta | Calorimetric and thermodynamic analysis of cowpea β-vignin: unveiling effects of seed germination on the conformation of a storage protein |
| **SATAC INVITED LECTURES** | | |
| SATAC IL 01 | N B Singh | Hydration of Blended cement in presence of nanomaterials |
| SATAC IL 02 | Namdeo Gajbhiye | Reactivity and Thermo–Magnetic Spin Glass transition of Nano-Ferrites by Thermal Analysis and Calorimetry |
| SATAC IL 03 | Arun Pratap | Crystallization Kinetics of Multi-component Metallic Glasses using Differential Scanning Calorimetry |
| SATAC IL 04 | Ranjit K Verma | Understanding thermooxidative stress on Indian mustard oil during heating in air and impact of turmeric doping |
| SATAC IL 05 | Ramesh L Gardas | Advanced Thermal Analysis of Ionic Liquids and Deep Eutectic Solvents for Sustainable Metal Recovery from Spent Batteries |
| SATAC IL 06 | Jitendra S Sangwai | Enhanced carbon capture efficiency through additive-infused and amine-functionalized $SiO_2$ nanoparticle formulations |

|  |  |  |
|---|---|---|
| **ICTAC & ITS INVITED LECTURES** |  |  |
| **Track 1** |  |  |
| IL 01 | Sohel Murshed | A Critical Appraisal of Nanofluids Research and Development |
| IL 02 | Ajaya Battarai | Exploring the Role of Aspartic Acid in Modulating Micellization Behavior of Cationic Cetyltrimethylammonium Bromide |
| IL 03 | Zhiwu Yu | The formation of free-standing 2D crystals from amphiphilic species, the effect of counter ions |
| IL 04 | Alfréd Kállay-Menyhárd | Predictive structure-property correlations in semicrystalline polymers |
| IL 05 | Vilko Mandić | Innovative Techniques for Efficient Synthesis of Amorphous Nanoscale<br>Materials for Ultrafast Thermal Analysis |
| IL 06 | Amalendu Pal | Aggregation Behaviour of Amphiphiles in Aqueous Solutions of Various Additives |
| IL 07 | Dilip Dagade | Water in Solvation Shell of Ionic Liquids: Thermodynamic, NIR Spectroscopic, Molecular Dynamics and DFT Investigations |
| IL 08 | Amiya Panda | Thermodynamic analysis on the ionic liquid induced aggregation behavior of bile salts: An isothermal titration calorimetric approach |
| IL 09 | Eswarmoorthy Muthusamy | Solar Thermoelectric Generator with Flexible Thermal Storage |
| IL 10 | Surianarayanan Mahadevan | Significance of measuring metabolic heats in bioprocess monitoring |
| IL 11 | M Hamsa Priya | Peptide Self-assembly -- A Hydrophobic Collapse? |
| IL 12 | Santosh Deosarkar | Thermodynamic properties for understanding the molecular interactions in aqueous solutions of biomolecules and drugs |
| IL 13 | Pardha Saradhi Maram | Structure and Thermochemistry of Functional Metal Oxides |
| IL 14 | Riyazuddeen | Effect of molecular solvents on properties of imidazolium ionic liquid: Experimental and computational studies |
| IL 15 | Rama Nand Rai | Phase diagram, Thermal, Structural and Optical Studies of newly synthesized Co-crystals |
| IL 16 | G. Venkatarathnam | Recent developments to the Density marching methods for phase envelopes |
| **Track 2** |  |  |
| IL 17 | Kogularasu Sakthivel | Eco-innovative electrochemical sensing for precise detection of vanillin and sulfadiazine additives in confectioneries |
| IL 18 | Kothandaraman Ramanujam | High Capacity Aqueous Redox Flow Battery |
| **Track 3** |  |  |
| IL 19 | Kamalika Sen | Graphene Based Nanocomposites for Ultra-trace Sensing |
| IL 20 | Sujata Mandal | Thermal and Calorimetric Analyses in the Research and Development of Flame-Retardant Materials |
| **Track 4** |  |  |
| IL 21 | Pannuru Venkatesu | Ionic Liquids as green solvents for enhanced stability of proteins against multiple stresses |
| IL 22 | Dip Saikia | A review on the water absorption behavior of natural fibers |

| | | |
|---|---|---|
| IL 23 | Anima Nanda | Harnessing Green Nanotechnology for Industrial Solutions to Combat Antimicrobial Resistance |
| IL 24 | Mahesh B | An insight into synthetic polypeptide-based blends with other polymers: Emerging trends and advances |
| IL 25 | Sathyanarayana N. Gummadi | Lignocellulosic Biomass to Value Added Products: Xylitol production |
| **Track 5** | | |
| IL 26 | Kinga Pielichowska | Thermal properties of thermochromic organic face change materials for thermal energy storage |
| IL 27 | Debashis Chakraborty | Our latest polymer technologies for combating climate change |
| IL 28 | Hema Chandra Kotamarthi | Characterizing the oligomerization process of the proteasomal complex from Mycobacterium Tuberculosis |
| IL 29 | Jayaramulu Kolleboyina | Hybrid Two-dimensional Porous Materials |
| IL 30 | Yamini Sudha Sistla | Development of Biopolymer Based Food Packaging Films with Improved Moisture Barrier and Mechanical Properties |
| **Track 6** | | |
| IL 31 | Sarma Pisupati | Greener Critical Mineral Extraction Methods for Sustainable Energy to Mitigate Climate Change |
| IL 32 | Poonguzhali Elamvazhuthi | Phytochemical Extraction of Heavy Metals (Cd & Hg) Using Orange Peel / Turmeric Powder |
| **Track 7** | | |
| IL 33 | Sumit Bhawal | Gleanings from the synthesis of non-natural Thiamine analogues to develop novel anti-infectives |
| IL 34 | Naved Malek | Thermo-Responsive Multifunctional Ionic Liquid based Hydrogel as the New Age Drug Delivery Vehicles for the Treatment of Breast Cancer |
| IL 35 | Paurnima Talele | Calorimetric and spectroscopic approach to evaluate solid lipid nanoparticles-based drug delivery systems |
| **Track 8** | | |
| IL 36 | Dimitrios Bikiaris | Assessing Microplastics Mass Concentration in the Environment by Pyrolysis–Gas Chromatography / Mass Spectrometry |
| IL 37 | Deepak Kumar Ojha | Application of thermal analysis in the development of biomass valorization technologies |
| IL 38 | Meena Bisht | Uncovering the potential of aqueous solutions of deep eutectic solvents on the extraction and purification of collagen type I from Atlantic codfish (Gadus morhua) |
| IL 39 | Gaurav Pandey | Powering Tomorrow: Innovative Gas Hydrate Technologies for a Sustainable Future |
| IL 40 | Rajnish Kumar | Making CO 2 Capture and Sequestration one of the Most Sustainable Path for<br>Net Zero World |
| **Track 9** | | |
| IL 41 | Arun Tangirala | Creating and Including Open Educational Resources in the Era of Digital Education and Outreach |
| IL 42 | Edamana Prasad | Learning How to Teach |

| | | |
|---|---|---|
| **Track 10** | | |
| IL 43 | Sinjan Choudhary | Application of thermodynamics for discovery of potential inhibitors for disease associated protein targets |
| IL 44 | Arvind Kumar | Ionic Liquids and Deep Eutectic Solvents: Applications in Materials Chemistry and Biomass Processing |
| IL 45 | Homendra Naorem | Towards Development of Aloe Vera Based Hydrogel Iodophors as Antiseptic Agents: A Reappraisal |
| IL 46 | Sudhakar Dhondge | Solvation Behavior of Some Bioactive Compounds in Aqueous and Aqueous Solutions of Dextrose and Urea Solutions |
| IL 47 | Tamal Banerjee | Deep Eutectic Solvents as Novel Thermal and Separation Media: Insights from Quantum Chemical and Molecular Dynamics Simulations |
| IL 48 | Md. Sayem Alam | Effect of Additives on the Solution Behavior of Surfactants |
| IL 49 | Sangesh Zodape | Unveiling the Molecular Interactions of Ionic liquids and Drugs in aqueous Solutions through Volumetric and Compressibility Insights |
| IL 50 | Sushma Ijardar | Fundamentals and Applications of Aqueous Biphasic Systems Composed of Deep Eutectic Solvent |
| IL 51 | Vickramjeet Singh | Thermodynamics and Wetting of Aqueous Solutions of Benign Solvents |
| IL 52 | Ashwani Kumar Sood | Influence of environment friendly solvents and polymers upon the chemical and surface properties surface active agents for their industrial applications |
| IL 53 | Poonam Patyar | Thermophysical and FTIR properties of protein model compounds in aqueous Ionic Liquid solutions |
| IL 54 | Ranjan Dey | Green Solvents of the Future: Towards a Sustainable alternative |
| IL 55 | Ranjit K Verma | Role of thermal analysis in convenient accomplishments of useful magnetic, electrical and photoluminescent characteristics in ferrites, aluminates and chromites: a comparative account |
| **INDUSTRY TECHNICAL SESSIONS** | | |
| Slot 01 | Tadashi Arii | Simultaneous thermal analysis - mass spectrometry system with two types of interface structures and its applications |
| Slot 02 | Manohar Rao | Advancements in hyphenated techniques and thermal instruments |
| Slot 03 | Padmanabhan Govindarao | Thermal Conductivity Assessment - An innovative approach |
| Slot 04 | Rajdip Roy | RSC: Building community |
| Slot 05 | R Rajganesh | Advanced Thermal Analysis Techniques for the Characterization of Sustainable Polymers |
| **ORAL PRESENTATIONS** | | |
| **Track 1** | | |
| OP 1 | Anna Vykydalová | The study of carbon-epoxy laminate with novel flame retardants by cone calorimetry |
| OP 2 | Leo Kamiya | Phase Equilibria and of Structure II Clathrate Hydrate Formed with $CO_2$+Cyclohexanone |
| OP 3 | Chen-Rui Cao | Thermal analysis and calorimetric comparison of Taiwanese solid recovered fuels across seasonal variations |
| OP 4 | Aniket Arun Dhavale | Advancements in Heat Transfer: Metal-Foam Tube Banks for Compact Refrigeration Systems |

|  |  |  |
|---|---|---|
| OP 5 | Durgesh Srivastav | Comparative Numerical Analysis of Thermal Performance of various Cylindrical Li-ion Cells used in Electric Vehicle Battery Pack with Air, PCM and PCM-Fin-Based Cooling |
| OP 6 | Mitsuru Satoh | Characterization of the hydrate formed in the water + ethanol + carbon dioxide system |
| OP 7 | Ryonosuke Kasai | Crystal Growth and Morphology of $CO_2$ Hydrate with Sodium Chloride Aqueous Solution |
| OP 8 | Ion Mitsui | Thermophysical properties of thermal energy storage medium for battery cooling: Thermophysical properties of 2,5-dimethyl-2,5-hexanediol hydrates |
| OP 9 | Ajeet Kumar Srivastav | Thermogravimetric analysis of hydrated vanadium oxide nanostructures |
| OP 10 | Chandrashekhar Pandhurnekar | Solvation Behavior of Antidepressant Duloxetine Hydrochloride with Aqueous Myo-Inositol and different Amino acids solution |
| OP 11 | Santosh Kumar Bindhani | Effect of Temperature and composition on thermophysical properties of Binary liquid mixtures of Propiophenone with Propyl acetate, n-Butyl acetate and n-Pentyl acetate |
| OP 12 | Ajit Kumar Parwani | Comparative analysis of cooling methods in wire arc additive manufacturing of steel plate |
| OP 13 | Debayan Bhowmick | Double Diffusive Natural Convection within a Partially Saturated Porous Cavity Separated by a Wavy Interface: A Local Thermal Non-Equilibrium Approach |
| OP 14 | Kamlesh Parmar | Effects of Inclination on Thermal Performance of Closed-Loop Pulsating Heat Pipes |
| OP 15 | Arnab Lahiri | Interfacial Thermal Characteristics of a Composite Medium Subjected to a Short Pulse Laser Source |
| OP 16 | Chandradip Kumar Yadav | Effect of Percentage of Methanol on Micellization Position of Mixed Surfactant Dye Interaction |
| OP 17 | Noel Sam | Numerical Study on Heat Distribution And Effect Of Burner Configuration In Plate Conveyors |
| OP 18 | Pratiksha P. Gavhane | Thermodynamic Studies of Energetics of Ionic Interactions for Aqueous Choline Carboxylate Bio-ionic liquids at 298.15 K |
| OP 19 | Damanbha Marwein | Designing and developing an intelligent control system to be applicable for different heating and cooling applications |
| OP 20 | Deepak Kumar | Effect of Zinc Additive on Thermal Transport Properties of Novel Multicomponent Chalcogenide Se-Te-Sn System: Transient Plane Source Technique |
| OP 21 | Deepak V M | Thermodynamic model for pressure evolution during in-flight active pressurisation of liquid hydrogen tank of a cryogenic upper stage |
| OP 22 | Anu Jain | Exploring properties of protein fibrils from self-assembly to drug delivery: Thermodynamic analysis |
| OP 23 | T Srinivasa Krishna | Investigation of molecular interaction between 1-butyl-3-methyl-imidazolium hexafluorophosphate with Propyl acetate |
| OP 24 | Brajesh Kumar Ahirwar | Unlocking Efficiency: A Comprehensive Review of Advanced Techniques for Optimizing Solar Air Heater |
| OP 25 | Gizelle Rodrigues | Thermal performance analysis of an oval double-pipe heat exchanger in a porous medium using finite volume method |
| OP 26 | Sanjay H. Panjabi | Enhanced Micellization and Structural Transformation in Morpholinium-Based Ionic Liquids with Aromatic Counterions |

| | | |
|---|---|---|
| OP 27 | Insha Akbar | Deciphering the binding interactions of anti-cancer drugs using spectroscopic techniques and in-silico studies |
| OP 28 | Kaushal Kumar Sarswat | Studying the Mayer-Neldel rule and crystallization kinetics in STSI glassy systems using iso-conversional approaches |
| OP 29 | Krittika Patwari | Analysing the thermohydraulic performance of a double pass solar air heater integrated with triangular grooves |
| OP 30 | Md. Jamil Akhtar | Thermal management analysis of electric vehicles using low GWP refrigerants |
| OP 31 | Mihir Pandya | Electro-Thermal Analysis of single LFP Cell |
| OP32 | N. Hari Krishna | Thermophysical Properties, FT-IR and Computational studies on molecular interactions of Chlorobenzene with isomeric cresols |
| OP 33 | Narendra Kolla | Excess thermodynamic study of binary mixtures of Benzyl alcohol with amides over entire miscibility range ($0 < x < 1$) at temperature 298.15 - 323.15 K |
| OP 34 | Pinki mahur | Adsorption of amino acid on gold nanoparticles: a thermodynamic study |
| OP 35 | Ardila H. Tiwikrama | Carbon dioxide capture with ionic liquids and deep eutectic solvents: a new generation of sorbents |
| OP 36 | Brajesh Kumar Ahirwar | An updated Review on the Application of Nanofluids in several types of Heat Transfer Devices |
| OP 37 | Hrishikesh Sarma | Formulation of Nanofluids based on Natural Deep Eutectic Solvents |
| OP 38 | Pintu Purkait | Investigation of phase equilibria on LiCl-$LaCl_3$ binary system |
| OP 39 | Shantanu Dutta | Thermo-Hydraulic Behavior of Non-Newtonian Fluids in Mixed Convection within an Open-Boundary Square Duct Featuring an Embedded Adiabatic Block |
| OP 40 | Sajal Ghosh | Investigation of phase equilibria on LiCl-KCl-$LaCl_3$ ternary system |
| OP 41 | R Santhosh | Study on heat capacity of nickel - titanium - copper shape memory alloys |
| OP 42 | Pramod Ranjan Dash | Sustainable Transformation: Green Synthesis of Reduced Graphite Oxide via Thermal Reduction |
| OP 43 | Saukhya Telge | Investigation of porous metal foam enhanced PCM-based BTMS for CubeSat applications |
| OP 44 | Rajamohan Ganesan | Experimental Study of Natural Convection Heat Transfer in Horizontal Fin Arrays |
| OP 45 | S Shyam Kumar | Thermodynamic studies on Gd-Te system |
| OP 46 | Vishnu Saraswat | Multifaceted Characterization of Zinc-Doped Chalcogenide Glasses: Unveiling the Impact on Thermal, Mechanical, and Electrical Properties |
| OP 47 | Soujanya P | Investigating the Dynamics of Shock Wave and Flame Interactions |
| OP 48 | Tammisetty Ankaiah | Density, Speed of Sound, Refractive Index, FT-IR and computational studies of binary systems of ethyl lactate with 1-heptanol, 1-octanol, 1-nonanol at T = (298.15 – 323.15)K |
| OP 49 | Umamaheswari S. | Enhancement of Heat Transfer with Spinel-Type Ferrite Magnetic Nanofluids Under External Magnetic Fields |
| OP 50 | Vichitra Malaiyarasan | Thermal stability of monoethanaol amine based Deep Eutectic Solvent for different molar ratio |

| | | |
|---|---|---|
| OP 51 | Vishnu Saraswat | Thermal Study of Advanced Phase Change Materials with Zinc as a Chemical Modifier |
| OP 52 | Solaimalai Raja R | Thermophysical Properties Study on Composite Phase Change Material for Energy Recovery Applications |
| OP 53 | Bipin Kumar | Heat transfer and entropy generation in a heat exchanger tube carrying double perforated twisted tape with v-winglets |
| OP 54 | Amogh S Amblihalli | Longitudinal Vortex Generation using Various Winglet Configurations in Double-Pipe Heat Exchangers |
| OP 55 | Ansalin Gnana Sowndarya | Study of Inorganic carbonate-based flame-retardants for leather application: special focus on thermal characterization |
| OP 56 | Garima Bharti | Modeling and Efficiency Analysis of $SCO_2$ Recompression Cycle with Axial Flow Turbine Using Aspen HYSYS |
| OP 57 | Arumuga Perumal D | Effects of nanofluid flow rate and thermal conductivity on the response time of heat spreader integrated microchannel heat sink |
| OP 58 | Pratyush Anand Burnwal | Thermal characteristics of tubular energy storage system |
| **Track 2** | | |
| OP 1 | Nobuyoshi Koga | Intrinsic Hydration Kinetics of Inorganic Salts: A Case of $Li_2SO_4$ |
| OP 2 | Tibor Dubaj | Thermal decomposition of polymer blends: A direct mathematical deconvolution of thermogravimetric curves |
| OP 3 | Benson K. Money | Mixed Alkali Effect on Crystallization Kinetics of Lithium Metaphosphate Based Solid Electrolyte Glassy Systems |
| OP 4 | Anusha Gururajan | Pyrolysis of sesame stalk using non-isothermal thermogravimetric analysis:Thermo-kinetic studies using model-fitting and model free method |
| OP 5 | Ali Hodroj | A predictive multiple-distribution DAEM modeling of the impact of embedded salts on bitumen thermal behavior |
| OP 6 | Shubhro Chakrabartty | Development of a $TiO_2$ Nanoparticle Coating-Based Plasma Torch for Eco-Friendly Disposal of Municipal Solid Waste |
| OP 7 | Bibari Boro | Pyrolysis of waste printed circuit board: kinetic analysis and detail product characterization |
| OP 8 | Dasarath Maji | Study of σ → α phase transformation kinetics of Fe-48.5 at.% V alloy by using DSC |
| OP 9 | Geeta Chaudhary | MOF-derived perovskite oxide SrTi1-xCoxO3-δ as anion-intercalated electrode material for supercapacitor |
| OP 10 | Govind Dubey | Thermal and Catalytic Liquefaction of Northeastern Indian Coals with Tetralin and Toluene: Kinetic Modelling, Mechanisms and Product Characterization |
| OP 11 | Hemavathi S | Evaluation of Cooling Effectiveness for Cylindrical and Prismatic Batteries Using Oil Immersion Cooling System |
| OP 12 | Khokan Sahoo | Pyrolysis of petroleum pitch: Thermogravimetric analysis and non-isothermal kinetics using the distributed activation energy model (DAEM) |
| OP 13 | Pritam Kumar | Co-combustion of Biochars: Thermogravimetric Analysis and Distributed Activation Energy Modeling |
| OP 14 | Pritam Bhat | Thermal Impact of PCM Thickness on a Cylindrical Li-ion Cell |
| OP 15 | Ramakrishna Baliepalli | Numerical investigation of the effect of thermal energy storage materials on the performance of solar updraft tower (SUT) integrated with natural and forced draught systems |

|  |  |  |
|---|---|---|
| OP 16 | Rishabh Mishra | Revealing the Augmentation of Surface Immobilization of Adsorbed Nickel Chalcogenate during Alkaline Water Oxidation |
| OP 17 | Shivaranjini S | Revolutionizing Sodium-ion Batteries: Efficient Ion Diffusion Analysis and State of Charge Prediction with Time Series Analysis |
| OP 18 | Venkatesan Subramanian | Impact of Injector Nozzle Variation on HCCI Engine Performance with Juliflora Biodiesel and Hydrogen Using Response Surface |
| OP 19 | Yuv Raj Sahu | Kinetics and Mechanism for Catalyzed Oxidation of Oxacillin |
| OP 20 | Eledathu Kuriachan Sachin | Thermal Decomposition and Kinetic Study of Chemically Treated Glass Fiber Reinforced Polymer Composites |
| **Track 3** |  |  |
| OP 1 | Jaroslav Barták | From Viscosity to Crystal Growth and Diffusion: A Comprehensive Study of Ge25Se75 Amorphous Material Prepared in Different Forms |
| OP 2 | Anil Kumar | Exploring dielectric and AC conduction characteristics in elemental selenium glass modified with silver halides |
| OP 3 | Ankur Bhansali | Experimental investigation of hybrid nanoparticles based eutectic phase change materials for efficient thermal energy storage |
| OP 4 | Seikh Asif | Graphene Quantum Dots as Ratiometric Fluorescent Sensor for Lactic Acid |
| OP 5 | Biswajit Dalai | Deep-Ultraviolet (DUV) nonlinear optical (NLO) crystals: An application in Photonic Technologies |
| OP 6 | Luis A. Pérez-Maqueda | Generalized interface reaction kinetic models for heterogeneous contracting processes |
| OP 7 | Nisha Kumari | Exploring Compensation Effect and Conduction Mechanism in Current-Voltage Characteristics for Binary ST system and Ternary STTM (i.e., doped transition metals Fe, Co, Ni, Cu) system |
| OP 8 | Sachin Kumar Yadav | Tailoring of Selenium Nanocomposite Properties: Unveiling the Role of rGO/Graphite in Dielectric, Mechanical, and I-V Characteristics |
| OP 9 | Shamjetshabam Sumitkumari Devi | A 2D Supramolecular Cu (II) complex with 4,4-diaminodiphenylsulphone: Synthesis, spectroscopic characterizations, crystal structure and its biological activities |
| OP 10 | Sreekumar E N | Fabrication and analysis of Aluminium based Metal Matrix Composite with Carbon Nano Tube (CNT) as reinforcement |
| OP 11 | Veeraraahavan R S | Specific heat measurement of refractory metals and their binary alloys at temperatures above 1500ºC |
| OP 12 | Priyanka Ghorpade | Optimizing Phosphonium-Based Ionic Liquid Electrolytes for Enhanced Supercapacitor Performance |
| **Track 4** |  |  |
| OP 1 | Darshit Upadhyay | Investigation of plasma pyrolysis system for different biomass: An experimental and thermodynamic study |

| | | |
|---|---|---|
| OP 2 | Ashi Dutta | Experimental Investigation of Polycyclic aromatic hydrocarbons (PAHs) Emissions from Gasoline Direct Injection Engines Using Biofuels |
| OP 3 | Arjun C P | Coal bottom ash as an effective catalyst for biomass gasification |
| OP 4 | Deepak Chahar | Impact of Acylthiourea Based Rhodium Complexes on Proteolytic Activity and Conformational Stability of α-chymotripsin |
| OP 5 | Kshetrimayum Sangeeta Devi | Green Synthesized Copper Oxide Nanoparticles Using Hedhycium rubrum, antimicrobial assay and anticancer assay against A549 and HeLa cell lines |
| OP 6 | Gurunathraj Elumalai | Optimization And Comparison Of Various Biodiesels Using Response Surface Methodology and Machine Learning Techniques |
| OP 7 | Darshit Upadhyay | Investigations of mineral wool type insulations on Improved Biomass Cookstove |
| OP 8 | Sunita Rajamani | Ionic liquids for energy production |
| OP 9 | Nagesh Babu Vemula | A Comprehensive Review on the Optimization of Emulsified Biodiesel-Fueled Engines Using AI and ML Techniques |
| OP 10 | Partha Sarathi Nial | Lanthanide-induced left-handed DNA: A biophysical and thermodynamics study |
| OP 11 | Sanasam Yaiphabi | Thermal properties analysis of silk fibroin biomaterial film prepared from Antheraea frithi Moore cocoon for potential biomaterial applications |
| OP 12 | Shalu Yadav | Effects of biogenic nanoadditives on diesel engine combustion, performance and emission characteristics |
| OP 13 | Shiv Prakash Dadhich | Modeling and simulation of a torrefaction gas filtration system |
| OP 14 | Spurthi Joanna Selladurai | Lattice Boltzmann Method comparison for the microneedles and hollow micro needles assisting TDD model |
| OP 15 | Umamageshwari Rajkumar | Isolation of Protease Enzyme from Fish Visceral Wastes and its Application in Leather Processing |
| OP 16 | K. Kamalakannan | The state of the art of the development of Zinc based biodegradable materials- A brief review |
| OP 17 | Vijayakumari.S | Crystallization kinetics to achieve Stoichiometric Combeite (Na2Ca2Si3O9) and Silicorhenanite (β-Na2Ca4(PO4)2SiO2) Single Phasic Bioactive Glass System |
| **Track 5** | | |
| OP 1 | Florian GIMENO | Thermal denaturation and aggregation of horn keratin observed by differential scanning calorimetry (DSC) |
| OP 2 | Ashish Desai | Precision in Laser Cutting of KFRP Composites: Insights from Taguchi and ANN-Based Techniques in Materials Engineering |
| OP 3 | Rajat Roy | Structural and Thermal Behaviours of Iron-based Gas Atomized Powders |
| OP 4 | P L Ramkumar | Thermal Analysis and Characterization of Natural Cellulosic Fiber from Azadirachta Indica and its Polymer Composites |
| OP 5 | Asharani Maisnam | Investigation on possible use of Aloe Vera or mixed Aloe Vera hydrogels with gelatin or HPC as Iodophors and the controlled release of Iodine from the hydrogels |

| | | |
|---|---|---|
| OP 6 | Potshangbam Sorodhoni Devi | Study on the use of Aloe Vera gel, Gelatin, or their co-gels as templates for entrapment of $Pb^{2+}$, $Cu^{2+}$, or $Fe^{2+}$ from their aqueous solutions |
| OP 7 | Thoudam Chanchan Devi | Investigation on structural properties, thermal stability and photoluminescence properties of biocompatible Eu (III) doped calcium phosphate nanoparticles |
| OP 8 | Prashant Khanna | Evaluating the Optimal LLDPE/NaOH-Treated Peanut Shell Powder Blend for Improved Rotational Molding Processability |
| OP 9 | Keerthana A | Kinetic Analysis and Pyrolysis Behaviour of Polydimethysilane using Evolved Gas and Thermal methods |
| OP 10 | Devanshu Pathak | Covalent modification of Cellulose for selective extraction of Mercury ($Hg^{2+}$) and Lead ($Pb^{2+}$) |
| OP 11 | Mansingh Yadav | Effect of Yttria Concentration on the Mechanical and Thermal Stability of Yttria Stabilized Zirconia (YSZ): First Principles Studies |
| OP 12 | Nabila Tabassum | Assessing the Structural, Mechanical and Thermal Properties of AlCoCrFeNi High Entropy Alloy for High Temperature Applications: Atomistic Simulations |
| OP 13 | Omish Sethi | Thermally Stable, Mechanically Robust and Highly Conducting Eutectogels as Electrolytes for Supercapacitors |
| OP 14 | Laishram Peter Singh | Synthesis of highly luminescent $Eu^{3+}$ and $Tb^{3+}$-doped hexagonal-phase YPO4 nanoparticles with tunable emission at ambient temperature |
| OP 15 | Anat Ram Sidar | Synthesis of Hydrogen Bonded Copper(II) Coordination Polymer: Photocatalytic Degradation of Rose Bengal Dye and Luminescent Sensing of $Hg^{+2}$, $Cr_2O_7^{2}$, and Nitrofurantoin |
| OP 16 | Priyadharshini D | Transforming biowaste Calotropis procera pappus into superhydrophobic material for organic solvent/oil-water separation |
| OP 17 | Rashmi Prabha | Characterization of conjugate between poly (N-vinyl caprolactam) and triazine-based covalent organic framework as potential biomaterial |
| OP 18 | Sangamesh Suligavi | Investigation on the Performance of Nanofiber Coated Filter Media for Engine Applications |
| OP 19 | Sanjay Mor | Unravelling the role of Gold nanoparticles modified by using ionic liquids having different anions on phase transition behaviour of PNIPAM-b-PACMO |
| OP 20 | Tauseef Yazdani | Mitigating hydrogen embrittlement in AHSS DP980: Efficacy of Nickel-Chromium coatings in preserving mechanical properties |
| **Track 6** | | |
| OP 1 | Srinivasan Latha | Batch adsorptive Removal of Copper (II) from aqueous solution by chitosan oligosaccharide - nanocrystalline cellulose-g-AM hydrogel composite |
| OP 2 | Ajit Kumar Parwani | Development of Carbon Dioxide Capture unit for Diesel Engine |
| OP 3 | Sinchan Hait | Examining $CO_2$ Capture in Hydrophobic Natural DES: Thermodynamic Properties and Environmental Screening |
| OP 4 | Swathi Chenna | Green Methods for Sustainable Zinc Metal Ion Extraction from Water Sources |

| | | |
|---|---|---|
| **Track 7** | | |
| OP 1 | Kohsaku Kawakami | Crack or Nuclei? What happens for pharmaceutical glasses annealed at low temperature? |
| OP 2 | Debashree Das | Thymol encapsulated β-cyclodextrin for enhanced bio-efficacies |
| OP 3 | Tridib Banerjee | Effect of chitosan coating on liposomal encapsulation of cisplatin in a thin film hydration method |
| OP 4 | Swapnali S. Desai | Thermodynamic Investigation of Molecular Interactions for Biosensing of Creatinine using β-cyclodextrin |
| OP 5 | Sadaf Fatima Syed | Inhibiting the activity of mature Plasmepsin II from Plasmodium falciparum using fluoroquinolone-based antibiotics: Biophysical approach |
| OP 6 | Sunil Meena | Application of DSC and TGA in exploring the temp induced changes in food and dairy products |
| **Track 8** | | |
| OP 1 | Ayisha Fahmi K P | Investigation of Calorific Values and Thermal Degradation Profiles of Various Plastic Wastes |
| OP 2 | Rohit Kumar Dev | Synthesis and characterization of novel cetyl pyridinium chloride amino acid-based ionic liquids |
| OP 3 | Kavithakani A | Process optimization and modelling for the ozonolytic degradation of Atrazine |
| OP 4 | Loganathan T | Design and Development of Sustainable Sports Shoes Using Recycled Materials in Compliance with Testing Standards |
| OP 5 | Nikhil Dev | Evaluation of Combustion Quality Index Using Graph Theory and Matrix Method |
| OP 6 | Pranav Gupte | A theoretical exploration into the associations among enablers and sustainable manufacturing technologies |
| OP 7 | Pratibha Sharma | Investigating the effect of temperature on carbon dioxide adsorption capacity of amine-modified clay |
| OP 8 | Rajesh Chengamchetty Murali | Development of Leather Waste Composite Sheets as Sustainable Material for Upholstery Applications |
| OP 9 | Sachind Prabha Padinhattath | Extractive Removal of Dyes from Industrial Effluent: A Circular Approach Employing Pseudoprotic Ionic Liquids |
| OP 10 | Srinivasarao Kancharla | Solid Phase Recovery of Valuable Metals from Electronic Waste |
| OP 11 | Vibhav Shukla | Fe-doped Zinc-MOF Composites and its Test-Strip Employed for Colorimetric Detection of Glucose in Model and Real Urine Samples |
| OP 12 | Arumuga Perumal D | Numerical analysis of $LiFePO_4$ battery wall temperature with air cooling using copper metal foam |
| **Track 10** | | |
| OP 1 | Shikha Indoria | Volumetric Studies of Theophylline-PEGylated Deep Eutectic Solvent in Aqueous Solution |
| OP 2 | Nishaben Desai Dholakiya | Thermophysical Properties of Arabian sea for Feasibility of Desalination Plants in Estuarine Systems |
| OP 3 | Praseeda P Nair | Intermolecular interaction studies of DMSO/NMP+Water Systems at varying temperatures |
| OP 4 | Suraz Kumar | Thermophysical properties of DES, Glyceline with C2-C4 alcohols at varying temperatures |

## POSTER PRESENTATIONS

### Track 1

| | | |
|---|---|---|
| PP 01 | Srikanth Divi | Dielectric Response of Solvents Using Molecular Simulations |
| PP 02 | Anoop Kishore Vatti | Thermal Conductivity and Stability of Cyrene Nanofluid using Molecular Dynamics Simulations |
| PP 03 | Bhosale Bajrang | Investigation of component interaction in aqueous solution of Nicotinic acid solutions inpresence of L- Serine: Volumetric, Acoustical, Viscometry and Optical properties studies. |
| PP 04 | Brahamdeo yadav | Determination of Critical Micelle Concentration (CMC) of Sodium Stearate Solution in Different Temperature |
| PP 05 | Tanujit Biswas | Novel observation of Negative heat capacity and Fragility threshold in AgI-Ag$_2$O-MoO$_3$ glass |
| PP 06 | Faraz P Junaid | Climate Chamber-Assisted Oil-Bath Calorimetry for Accurate Specific Heat Determination of Lithium-Ion Cells |
| PP 07 | Vandana Shende | Volumetric and compressibility studies of antimycobacterial drug in aqueous and aqueous D-glucose solutions at various temperatures |
| PP 08 | Rohidas Vyankatrao Dudhate | Investigation of volumetric, optical and transfer properties of ascorbic acid with different cosolutes at 303.15 K |
| PP 09 | Atmaram Arsule | Density and Utraacoustic Properties of Antibacterial Pyridoxine Hydrochloride and Neomycin Sulphate Drugs in Aqueous Carbamide Solutions at Different Temperatures |
| PP 10 | Hrishikesh Pawar | Partial molar volumes, compressibilities and viscosities of Ranitidine Hydrochloride in aqueous-NaCl/sucrose solutions at 303.15 K |
| PP 11 | Julfikar Hassan Mondal | Thermophysical properties of a newly synthesized cationic surfactant |
| PP 12 | Malik Riahan Ahmad | Thermodynamic, transport and structural studies of Imidazolium Ionic liquids and Molecular solvents mixtures at (298.15 to 323.15) K and 0.1 MPa |
| PP 13 | Sanjay Panjabi | Enhanced Micellization and Structural Transformation in Morpholinium-Based Ionic Liquids with Aromatic Counterions |
| PP 14 | Nibedita Samanta | Influence of PbO on thermal behaviour of boro-tellurite glasses |
| PP 15 | Anupama Rai | Biophysical Study to Investigate the Interaction of some of aminoglycosides with Mycobacterium tuberculosis G-quadruplex DNA |
| PP 16 | Bala Karuna Kumar Doupati | Investigation of Molecular Interactions by Volumetric, Ultrasonic, Spectral and Computational Studies in Selected Binary Liquid Mixtures of 2-Chloro Ethanol over the Temperature Range 298.15 - 323.15 K |
| PP 17 | Aswini A | A study on thermophysical, physiochemical, and surfaces properties of fatliquors |
| PP 18 | Ion Mitsui | hermophysical properties of thermal energy storage medium for battery cooling: Thermophysical properties of 2,5-dimethyl-2,5-hexanediol hydrates |
| PP 19 | Bignya Rani Dash | Impact of Carboxylate Anion Chain Length and Temperature on Physicochemical Properties of Butyrolactam based Protic Ionic Liquids. |

|  |  |  |
|---|---|---|
| PP 20 | Chi-Min Shu | The effects of natural environmental storage on the aging rate and thermal hazard characteristics of firecrackers |
| PP 21 | Chen-Rui Cao | Effects of adding various ionic liquids on the inflammability and thermal stability of industrial oils |
| PP 22 | Aarzoo Ahuja | Thermo physical study on binary mixtures of Furfural and n-butyl acetate or isobutyl acetate or tert-butyl acetate at 298.15, 303.15 and 308.15 K. |
| PP 23 | Rachana Singh | Experimental, theoretical and spectroscopic analysis of molecular interactions in binary liquid mixtures comprising 4-methyl-2-pentanol + CmH2m+1OCH2CH2OH (m = 2,3,4) at different temperatures |
| PP 24 | Prerna Yogeshwar | Environmental sustainability and economic viability of Phase Change Materials |
| PP 25 | Tangeda Savitha Jyostna | Thermodynamic and DFT studies between 1, 2-ethylenediamine and 1, 5-Pentanediol at T = (293.15 to 313.15) K |
| PP 26 | Vandana Patel | Analysing the molecular interactions of KCl in 0.05 mol.kg$^{-1}$ aqueous 1-methyl -3 Propylimidazolium Iodide at various temperatures through physicochemical studies |
| PP 27 | Maddela Raji | Influence of methylene group and Effect of Temperature on Density, Speed of Sound, and Viscosity data of Haloarene with Linear alkanes |
| PP 28 | Ankita Chandak | Exploring the Solvation Behavior of D-Glucose in Aqueous Imidazolium-based Ionic Liquid Solution at different Temperatures |
| PP 29 | Rizos-Evangelos Bikiaris | Thermal properties of modified chitosan-based sponges with enhanced haemostatic properties for wound healing applications |
| PP 30 | Rupesh Kumar Pradhan | Exploration of interactions between L - Aspartic acid and Saccharides in aqueous medium at T= (293.15-313.15) K: Physicochemical and Spectroscopic approach |
| PP 31 | P. Shyamala | Kinetic and thermodynamic parameters of reactions in reverse micelles |
| PP 32 | Guruprasad Hasolkar | Thermodynamic Studies of Ionic Interactions in Aqueous Solutions of Diethylammonium based Protic Ionic Liquids |
| PP 33 | Haruka Abe | Observation of the α-β phase transition of quartz by differential scanning calorimeter |
| PP 34 | Indrajit Das | Alternative Solvents for Efficient $CO_2$ Capture: The Role of Basicity, Free Volume, and their Thermodynamic Properties |
| PP 35 | P. Annapurna | Exploration of volumetric, optical, thermodynamic, FT-IR and DFT studies of binary mixtures of ethanoic acid with higher 1-alkanols at different temperatures |
| PP 36 | Pranali Umredkar | Physicochemical Properties of Biogenic Monoamine Neurotransmitters: Volumetric, Viscometric and Thermoacoustic Investigations |
| **Track 2** |  |  |
| PP 01 | Sunita Rajamani | Ionic liquids as a dual solvocatalyst for esterification reactions |
| PP 02 | Somenath Panda | Stability of Current Collectors in Ionic Liquid Electrolytes for Aluminum-Ion Batteries |

| | | |
|---|---|---|
| PP 03 | Kondepogu Devaiah | Redox Active Deep Eutectic Solvents (DES) For Energy Storage |
| PP 04 | Vipul Ghare | Investigating the Effect of Nd$^{+3}$ Substitution on the Supercapacitor Performance of Cobalt Copper Ferrites |
| PP 05 | Vikas Kumar | Full solar spectrum active Fe-doped CuSe nanostructure for enhanced photocatalytic activity: Structural, optical and photocatalytic performance investigation |
| PP 06 | Vipin Kumar | Adsorption of D-A’-π-A Carbazole dyes on $TiO_2$ surface for Dye-Sensitized Solar Cell Applications |
| PP 07 | Praful Jambhule | Comparative study of photocatalytic degradation of dye using $Fe_3O_4$ using electromagnetic radiations of various energies |
| PP 08 | Diksha Praveen Pathak | A Computational Study on Transition metal doped MOF-5 for Carbon Capture |
| PP 09 | Matko Erceg | Kinetic analysis of the non-isothermal decomposition of PEO10/25A/LiBOB polymer nanocomposite electrolytes |
| PP 10 | Luis Perez-Maqueda | Generalized interface reaction kinetic models for heterogeneous contracting processes |
| PP 11 | Manisha Chakraborty | Effect of Reaction Atmosphere on the Thermal Decomposition of Iron(III) acetylacetonate Leading to Iron Oxide Nanoparticles |
| PP 12 | Atsumi Miyake | Thermal stability of ammonia borane for alternative onboard hydrogen carrier |
| PP 13 | Mito Hotta | Water Vapor Effects on the Physico-Geometrical Consecutive Process of the Thermal Dehydration of Sodium Carbonate Monohydrate |
| PP 14 | Nobuyoshi Koga | Multistep Thermal Dehydration Kinetics of Geopolymer Pastes Prepared Using Different Active Fillers |
| PP 15 | Konstantinos Chrissafis | Enhancing Thermal Analysis Precision: Exploring Isoconversional Methods for Accurate Data Evaluation |
| PP 16 | Arpan Tewary | Enhancing Green $H_2$ Generation: The Role of Oxide-Nitride Interface Based Electrocatalysts |
| PP 17 | Harikrishna R B | Nanoporous Samarium and Cerium-Based Metal-Organic Frameworks for Enhanced Photocatalytic Water Splitting |
| PP 18 | Leela kumari Bodasingi | Kinetic study of the dissociation of $[Co(tpy)_2]^{2+}$: Comparison between AOT/Heptane and CTAB/Chloroform/Hexane reverse micellar environments |
| PP 19 | Shuto Yamada | Kinetics on the Thermal Degradation of Polyimide |
| **Track 3** | | |
| PP 01 | Rakesh Singh | Correlation between crystal structure parameters with optical, electronic, luminescent, and magnetic parameters of barium hexaferrite nanomaterials at controlled thermal temperature |
| PP 02 | Manoj Kumar Adhikari | Exploring the Protective Effects of Surfactants against Corrosion: A Comprehansive Review |
| PP 03 | Nadezda Malkova | Polyborazylene characterization: Determination of subsequent polymerization steps by DTA analysis |
| PP 04 | Haruka Abe | Specific heat capacity measurement of silica glass by differential scanning calorimeter |
| PP 05 | Rajasekar K | Green route synthesis, spectral characterization and crystal structure of $[Cd(4\text{-}AAP)_2(NO_2)_2]$ |

| | | |
|---|---|---|
| PP 06 | Somya Deep Dey | An analytical review of the current status and challenges in the development of inorganic phase change materials for thermal energy storage |
| **Track 4** | | |
| PP 01 | Ambika Kumaresan | Preparation and characterization of microencapsulated antimicrobial insock/footbed for foot comfort |
| PP 02 | Vijayakumari S | Crystallization kinetics to achieve Stoichiometric Combeite ($Na_2Ca_2Si_3O_9$) and Silicorhenanite ($\beta$-$Na_2Ca_4(PO_4)_2SiO_2$) Single Phasic Bioactive Glass System |
| PP 03 | Sweta Jha | Separation of 5-HMF from the Ionic Liquids Using Phenolic Solvents Using Molecular Dynamics Simulations |
| **Track 5** | | |
| PP 01 | Vincelet Jobikha A | Optical properties of $Dy^{3+}$ doped tin borophosphate glass for radiation shielding applications |
| PP 02 | Sangeetha D R | Superhydrophobic nanocomposites for coating leather and other surfaces |
| PP 03 | Anat Ram Sidar | Synthesis of Hydrogen Bonded Copper(II) Coordination Polymer: Photocatalytic Degradation of Rose Bengal Dye and Luminescent Sensing of $Hg^{+2}$, $Cr_2O_7^{2-}$, and Nitrofurantoin |
| PP 04 | Jaishree Sharma | Micro-textured ETFE for self-cleaning application |
| PP 05 | Bhimarao Patil | Investigating Caesium Immobilization in $BaAl_2Ti_6O_{16}$: Synthesis, Characterization, and Leaching Studies |
| PP 06 | Piotr Szatkowski | Evaluation of thermal properties of phase change materials modified with nanoadditives for solar energy harvesting applications |
| PP 07 | Kinga Pielichowska | Bio-based carbon aerogels infiltrated with sugar alcohols as shape stabilized phase change materials |
| PP 08 | Piotr Szatkowski | Enhancing the properties of phase change materials (PCMs) by carbon-based materials for electo-thermal conversion |
| PP 09 | Chaitanya Gandhi | Molecular Dynamics Simulations Study on Structural and Thermodynamic Analysis of Mixtures of Oxidized and Unoxidized Forms of Polyaniline |
| PP 10 | Johan Stanley Samuel Jayakaran | Synthesis and Characterization of Biobased multiblock copolymers: Poly(ethylene2,5-furandicarboxylate)- b -Poly($\varepsilon$-caprolactone) targeting food packaging applications. |
| PP 11 | Ignazio Blanco | Thermal Behavior of Low Density Polyethylene for Agricultural Applications |
| PP 12 | Dimitrios Bikiaris | Zwitterion-modified chitosan derivatives for dental applications: Synthesis and thermal properties characterization |
| PP 13 | Bindu Yadav | Unravelling the Stabilization Mechanism of Mono-, Di and Tri-Cholinium Citrate-Ethylene Glycol DESs towards $\alpha$-Chymotrypsin for Preservation and Activation of the Enzyme |
| PP 14 | Pooja Yadav P | Impact of imidazolium type Zwitter Ion Ionic Liquids on peroxidase activity and conformational stability of cytochrome c |
| PP 15 | Pooja Yadav | Enhanced Thermoresponsive Behaviour in MXene-Embedded PVCL Composites: Lowered LCST and Potential Biomedical Applications |
| **Track 6** | | |
| PP 01 | Pratap Chhotaray | Study of Novel Surfactant Based Spectroscopically Active Ionic Liquids |

|  |  |  |
|---|---|---|
| PP 02 | Yogendra Kumar Mishra | Nanoparticle assisted micro gelation enhanced carbon capture through modified amines using absorption from simulated flue gas stream |
| PP 03 | Ramanaiah Seella | Conversion of fruit waste (banana peels) into bioplastic and its degradation by soil microorganisms |
| **Track 7** |  |  |
| PP 01 | Bajrang Lal | Design, Synthesis, and Studies (Antimicrobial Activity, Molecular Docking, and DFT) of Ampyrone linked Bis-triazoles |
| PP 02 | Shaik Mahammad Rameez Arhan | Computational and Thermodynamic Analyses for Rapid Drug Repurposing: Insights into Viral Pandemics and Therapeutic Candidates |
| PP 03 | Nandini Dave | Synthesis and Antifungal Activity of Some Coumarin-based 1,2,3-Triazole Derivatives: A Review |
| PP 04 | Syed Tanweer Ahmed | Automation of thermal process safety information delivery |
| PP 05 | Rahul Gupta | Repurposing Fluoroquinolone Drugs for the Treatment of Actinopathy-Induced Neurodegeneration |
| **Track 8** |  |  |
| PP 01 | Athira K K | Extraction of DNA using Ionic Liquid-based Aqueous Biphasic System |
| PP 02 | M. Shaibuna | Effective Removal of Heavy Metal Ions using Hydrophobic Deep Eutectic Solvents |
| PP 03 | Baiju Chenthamara | Sustainable Metal Recovery from Spent Lithium-ion Battery Cathodes Using Deep Eutectic Solvents |
| PP 04 | Murugesan A | Solvent-Free Depolymerisation Methods for Sustainable Plastic Waste Recycling into Value-Added products for Material Application |
| PP 05 | Vibhav Shukla | Fe-doped Zinc-MOF Composites and its Test-Strip Employed for Colorimetric Detection of Glucose in Model and Real Urine Samples |
| PP 06 | Nikolaos Bikiaris | Biodegradable and sustainable PLA-based substrates destined for printed and flexible electronics |
| **Track 10** |  |  |
| PP 01 | Vahishta Katrak | Investigating Experimental and Theoretical Thermophysical Properties of Binary Systems of Deep Eutectic Solvents with Water |
| PP 02 | Nensi Patel | Designing Aqueous Biphasic Systems of Quaternary Ammonium Salt based Deep Eutectic Solvents in presence of Inorganic Salts |
| PP 03 | Anuja Jain | Elucidating Molecular Interactions of Imidazolium-Based Ionic Liquid in Aqueous and Aqueous Amino Acid Solutions: Volumetric and Compressibility Studies |
| PP 04 | Mustaqueem Shaikh | Apparent Molar Volumes and Apparent Molar Isentropic Compressibilities of Procaine/Tetracaine Hydrochloride in Aqueous Solutions at Different Temperatures |
| PP 05 | Sapna Warkari | Thermodynamic studies of maline (choline chloride + malonic acid) and ethanol based pseudo-binary mixture |
| PP 06 | Sneha Bankar | Delving into solutions of Azithromycin in 1,2-propanediol, DMSO and ethanol through ultrasonic, volumetric and viscometric properties analysis across a temperature range of 288.15 K to 318.15 K |

| | | |
|---|---|---|
| PP 07 | E A Lohith | Elucidation of molecular interactions in cyclohexanol with aniline and chloro substituted aniline binary mixtures in terms of spectroscopic and DFT study |
| PP 08 | Omish Sethi | Thermophysical and Electrochemical Properties of Natural Deep Eutectic Solvents (NADES): The Effect of Water Addition and Hydrogen Bond Donor Identity |
| PP 09 | V P Priyanka | Influence of Mono- and Di-cationic Ionic Liquids on Bile Salt Aggregation and Drug Interaction |
| PP 10 | K J Jisha | Investigating Hemoglobin Stability in DBU-Based Protic Ionic Liquids: A Spectroscopic Approach |

# Presentation Timelines

| Presentation | Duration |
|---|---|
| Robert Mackenzie Award Lecture (AL) | 60 min |
| The TA instrument-ICTAC Award Lecture (AL) | 50 min |
| Plenary Lecture (PL) | 45 min |
| Rigaku-ICTAC Young Scientist Award (AL) | 30 min |
| ICTAC Promising Researcher Award (AL) | 30 min |
| ICTAC Travel Grant Awards (AL) | 15 min |
| Invited Lecture (IL) | 25 min and 5 min Q&A |
| Short Invited Lecture (SIL) | 17 min and 3 min Q&A |
| Oral Presentations (Senior Researchers (OP-SO)) | 17 min and 3 min Q&A |
| Oral Presentations (Young Researchers (OP-YO)) | 13 min and 2 min Q&A |

# Guidelines for Presentations

## Poster Presentation

4 feet (height) X 3 feet (width)

## Oral Presentation

All Oral Presentations in the ICTAC 2024 will be delivered as part of a specific technical session. Each Oral Presentation by senior researchers will last for 17 minutes and 3 minutes Q&A by and by young researchers will last for 13 minutes and 2 minutes Q&A.

## Conference Organizing Committee

Convener : Ramesh L. Gardas, IIT Madras
Co-conveners : Jitendra S. Sangwai, IIT Madras
Ranjit K. Verma, Magadh University

## National Organizing Committee

Patron : V. Kamakoti, Director, IIT Madras
Chairman : Ranjit K. Verma, Magadh University
Secretary : Ramesh L. Gardas, IIT Madras
Jt. Secretary : Jitendra S. Sangwai, IIT Madras
Member : G. Sekar, Head - Chemistry, IIT Madras
Member : Niket S. Kaisare, Head - Chemical Engineering, IIT Madras

## *in Association with*

International Confederation for Thermal Analysis and Calorimetry
Indian Thermodynamics Society (ITS), Amritsar
Indian Chemical Society (ICS), Kolkata
Indian Council of Chemists (ICC), Agra

## International Advisory Board

## National Advisory Board

# Local Organising Committee

**Overall coordinators:**

Ramesh L. Gardas, CY-IITM
Jitendra S. Sangwai, CH-IITM
Ranjit K. Verma, Magadh University

**Registration Committee:**

Debashish Chakraborty, CY-IITM
Sooraj Kunnikuruvan, CY-IITM
Khusboo Suman, CH-IITM

**Accommodation Committee:**

Beeraiah Baire, CY-IITM
Mahiuddin Baidya, CY-IITM
Sagar Saurav, CH-IITM

**Transport Committee:**

T. Palani Selvam, CY-IITM
Sudam Dawande, CY-IITM
Md. Sayem Alam, CLRI

**Scientific Committee:**

Sanjay Kumar, CY-IITM
Dillip Kumar Chand, CY-IITM
Sankha Karmakar, CH-IITM

**Program Committee:**

Edamana Prasad, CY-IITM
Rajnish Kumar, CH-IITM
Y. Chaitanya Sharma, CY-IITM

**Hospitality Committee:**

R. Kothandaraman, CY-IITM
Sachin Gunthe, CE-IITM
Hemachandra Kotamarthi, CY-IITM

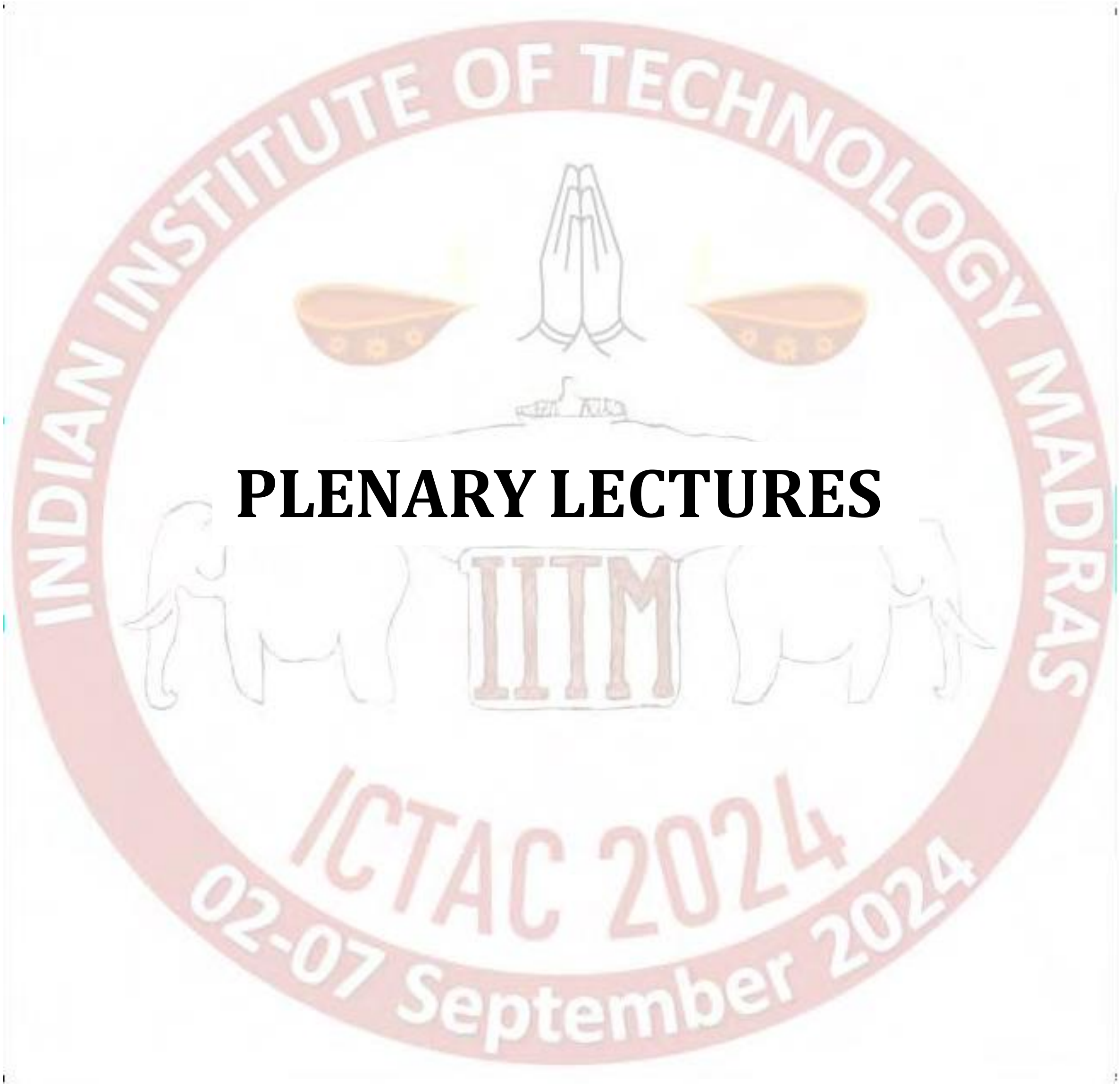
## Indian Thermodynamics Society Executive Committee

| | |
|---|---|
| Nand Kishore | Indian Institute of Technology Bombay, Mumbai |
| Tarlok Singh Banipal | Guru Nanak Dev University, Amritsar |
| Shantilal B. Oswal | Veer Narmad South Gujarat University, Surat |
| Homendra Naorem | Manipur University, Imphal |
| Ramesh L. Gardas | Indian Institute of Technology Madras, Chennai |
| Pannuru Venkatesu | University of Delhi, Delhi |
| Md. Sayem Alam | CSIR – Central Leather Research Institute, Chennai |

Amalendu Pal (Kurukshetra)
Renu Chadha (Chandigarh)
Sudhakar Dhondge (Nagpur)
Arvind Kumar (Bhavnagar)
A.K. Sood (Amritsar)
Dilip H. Dagade (Kolhapur)
Tamal Banerjee (Guwahati)
T. Savitha Jyostna (Warangal)
Ranjan Dey (Goa)
K. Sivakumar (Tirupati)

Poonam Patyar (Patiala)
Santosh Terdale (Pune)
Sushama Ijardar (Surat)
Naved Malek (Surat)
Tejwant Singh (Amritsar)
Vickramjeet Singh (Jalandhar)
Sinjan Choudhary (Mumbai)
Pratap Chhotaray (Bhubaneswar)
Meena Bisht (New Delhi)
Pooja Meena (Allahabad)

# PLENARY LECTURES



*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Methods based on the general rate equation – applications and limits

**PETER ŠIMON*, ZUZANA CIBULKOVÁ, TIBOR DUBAJ**

Department of Physical Chemistry, Faculty of Chemical and Food Technology, Slovak University of Technology, Radlinského 9, 812 37 Bratislava, Slovakia
*Corresponding author: e-mail: peter.simon@stuba.sk

**Keywords**: general rate equation, complex process, single-step approximation, thermoanalytical kinetics

Mechanisms of the processes in condensed phase are very often unknown or too complicated to be characterized by a simple kinetic model. They tend to occur in multiple steps that have different rates. To describe their kinetics, the rate of the complex multi-step condensed-state process can be formally described by the general rate equation (GRE).

In this paper, mathematical correctness and applicability of the methods based on the general rate equation, analyzed from the viewpoint of the new concept of understanding GRE as a formal mathematical tool [1], is presented. It is reasoned that the integral isoconversional methods, Kissinger method and the single-curve methods are suitable for the simple processes only and should not be applied in the thermoanalytical kinetics characterized by complex processes. No conclusions should be drawn from the values of individual kinetic parameters, particularly from the values of activation energy.

A special attention is devoted to the mathematically correct treatment of experimental data by the integral isoconversional methods [2]. Also, the methods based on the non-Arrhenian temperature functions are outlined [1].

Further, the meaning of the degree of conversion as defined in thermoanalytical kinetics is compared with the degree of conversion defined by IUPAC. It is shown that the physical meaning for both definitions may be significantly different.

**References**

[1] P.Šimon, T.Dubaj, Z.Cibulková, *J. Therm. Anal. Calorim*., (**2023**)
[2] T.Dubaj, Z.Cibulková, P.Šimon, *Thermochim. Acta*, 736 (**2024**) 179739.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# The generalized conversion functions for heterogeneous kinetics

**ANDREI ROTARU**[1,2]*

[1]Department of Engineering Science, Babeş-Bolyai University, Cluj-Napoca, Romania; [2]Department of Chemical Thermodynamics, Institute of Physical Chemistry–Ilie Murgulescu, Bucharest, Romania
*andrei.rotaru@ubbcluj.ro, andrei.rotaru@icf.ro

**Keywords**: heterogeneous kinetics, SB model, generalized conversion function.

Kinetic models are relevant to describe heterogeneous kinetic processes; a number of kinetic models and their mathematical expressions have been reported in the literature, many of these based on idealistic conditions in terms of geometrical constrain and driving forces. Alternatively, the semi-empirical Sestak-Berggren (SB) conversion function [1], which was proposed as a general equation, encompasses a large variety of equations corresponding to different kinetic models. Despite the fact that the SB equation does not provide any physical meaning, it is extremely useful for kinetic analysis as it offers a good fit to experimental data even when they do not follow the ideal conditions assumed for the conventional kinetic models [2]. Although the logarithmic part within the SB kinetic model is important (as in the case of historical kinetic models), it brings some impediments while playing the role of accommodation function at when $\alpha \to 0_+$ or $\alpha \to 1_-$. And last but not least, maybe the most important limitation is the fact that its conversion function cannot be analytically integrated to provide an exact solution; thus, it cannot be directly applied in kinetic integral methods.

In this study we aimed for a better understanding of the Sestak-Berggren generalized conversion function and proposed some solutions for certain specific cases [3], while the mathematical limits for the values of the kinetic exponents $m$, $n$, $p$ of the SB model and their validity were also explored [3]. Moreover, we have approximated the Sestak-Berggren (SB) conversion function with a new one (and also its consequent integral), which has the same behaviour and very important, the same extreme points of extreme (*i.e.* the maximum) [4]. Furthermore, an alternative for a superior conversion function – not related to the SB function – is also proposed [5].

## References

[1] J. Sestak, G. Berggren, *Thermochim. Acta*. 3(1) (**1971**) 1-12.
[2] J. Malek, J.M. Criado, J. Sestak, J. Militky, *Thermochimica Acta*. 153 (**1989**) 429-435.
[3] I. Rovenţa, L.A. Perez-Maqueda, A. Rotaru. *J. Therm. Anal. Calorim*. **(2024)**
[4] I. Rovenţa, A. Rotaru, L.A. Perez-Maqueda. *J. Therm. Anal. Calorim*. **(2024)** Submitted.
[5] A. Rotaru, I. Rovenţa. *Thermochim. Acta*. **(2024)** In preparation.

Acknowledgements: This work was performed in collaboration with Ionel Rovenţa (University of Craiova, Romania) and Luis A. Perez-Maqueda (Instituto de Ciencia de Materiales de Sevilla, Consejo Superior de Investigaciones Científcas − Universidad de Sevilla, Spain).

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermodynamic and Kinetic Perspectives to Monitor the Competition Between Decomposition and Vaporization in Ionic Liquids

**S. VECCHIO CIPRIOTI[1]*, J.M. SILVA FERRAZ[1], B. BRUNETTI[2], A. CICCIOLI[3]**

[1] Department of Basic and Applied Science for Engineering, University of Rome "La Sapienza",
Via del Castro Laurenziano 7, 00161 Rome, Italy
[2] ISMN-CNR, Department of Chemistry, University of Rome "La Sapienza",
P.le A. Moro 5, 00185 Rome, Italy
[3] Department of Chemistry, University of Rome "La Sapienza", P.le A. Moro 5, 00185 Rome, Italy
*Corresponding author: e-mail: stefano.vecchio@uniroma1.it

**Keywords**: thermal analysis, Knudsen effusion, thermal stability, ionic liquids

The well-recognized thermal stability of ionic liquids (ILs) [1], makes them suitable to be used, for example, as potential additive salts for battery electrolytes, improving the scarce thermal stability of the electrolyte, related to the use of flammable carbonate solvents. However, near ambient temperature at which most energy storage systems are expected to be utilized, the vapor pressure of ILs remains negligible (or at least not easily detectable), resulting in the non-flammability of these compounds. Furthermore, at ambient pressure many ILs are reported to be stable at least up to 200 °C.

Recently, several studies focused the attention mainly on the thermodynamics and kinetics of ILs vaporization [2], while others focused their attention on the elucidation of the competition between the occurrence of vaporization and decomposition [3]. These studies confirmed that ILs' thermal stability may be overestimated, especially if assessed only on the basis of the onset decomposition temperature from thermogravimetry (TG) [4].

Dicationic ionic liquids (DILs) are often recognized to be more stable than the corresponding ILs (with the same anion and comparable cation, except for the charge) because of its lower volatility. However, some examples were considered in which although DILs have lower vapor pressure than the analogues ILs in the same temperature range, their tendency to undergo thermal decomposition is considerably higher.

In addition, the extent of decomposition seems to depend considerably on the diameter of the effusion hole under effusion regime: the lower the diameter, the higher the extent of decomposition. Kinetic and thermodynamic factors were also discussed.

**References**

[1] B. Wang, L. Qin, T. Mu, Z. Xue, G. Gao, *Chem. Rev*, 117 (**2017)** 7113.
[2] M.I. Williams, J.S. Dickmann, M.E. McCorkill, J.C. Hassler, E. Kiran, *Thermochim. Acta*, 685 (**2020**) 178509.
[3] D.H. Zaitsau, A. Abdelaziz, *J. Mol. Liq*, 313 (**2020**) 113507.
[4] C. Ferdeghini, L. Guazzelli, C.S. Pomelli, A. Ciccioli, B. Brunetti, A. Mezzetta, S. Vecchio Ciprioti, *J. Mol. Liq*, 332 (**2021**) 115662.

# Structure-Property-Energetics Relationships in Deriving Guidelines for Rational Drug Design: Thermodynamic Approach

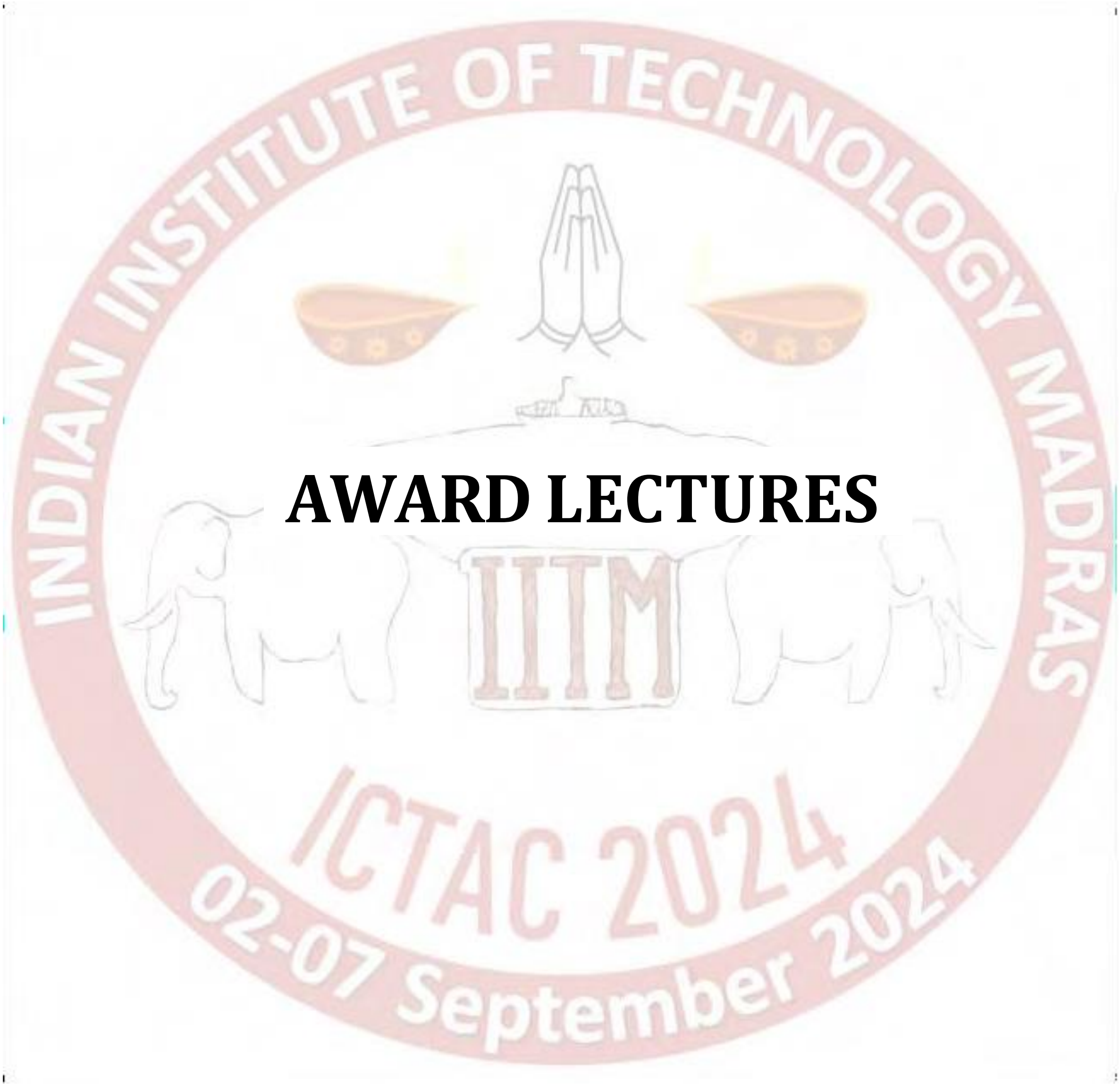
**NAND KISHORE***

Department of Chemistry, Indian Institute of Technology Bombay, Powai
Mumbai - 0400 076, India.
*Corresponding author: e-mail: nandk@chem.iitb.ac.in

Majority of synthetically developed new molecular entities or improved drug molecules have high hydrophobic content and low bioavailability. Therefore, suitable drug delivery vehicles are required for effective delivery of the drugs at the target site. Self-assembled colloidal structures such as micelles, niosomes, and liposomes offer an effective environment for drug encapsulation. We have quantitatively investigated partitioning of a variety of drugs varying from antibiotic, anticancer, anti-inflammatory and antithyroid into self- assemblies of cationic, non-ionic and mixture of cationic and non-ionic surfactant micelles, poloxamers, as well as of niosomes and their interaction with the transport protein serum albumin upon subsequent delivery. The effect of drug delivery vehicles on the thermal and structural stability of target protein have been investigated quantitatively. These studies have significance in understanding physical chemistry underlying partitioning of a variety of drug molecules into suitable delivery vehicles and permit establishing structure-property-energetics relationships.

Protein misfolding process is driven by formation of transient intermediates, which promote fibrillation/aggregation depending upon the primary sequence of the protein and environmental conditions causing neurodegenerative diseases such as Alzheimer’s, Parkinson’s, Huntington’s, diabetes, and Creutzfeldt-Jakob, amongst others. To revert amyloid fibrils to their native state is a challenge in finding a solution to prevent neurodegenerative diseases. We have adopted a structure–property–energetics correlation-based approach with molecular entities having diverse functionalities to explore their potential towards prevention of fibrillation in proteins and obtain mechanistic insights. We adopt quantitative comprehensive biophysical approach for identifying functionalities in molecules, which offers this feature in terms of polarity and hydrogen bonding. Our objective of identifying functionality on molecules that establishes effective intermolecular hydrogen bonding with β-strands of protein fibrils was achieved by combined calorimetric, spectroscopic, volumetric, and microscopic correlations. Detailed studies with osmolytes, drugs and ionic liquids have enabled identification of functionalities on the molecules capable of interfering in the association process and pushing the protein towards its native conformation. Thermal stabilization of proteins has direct correlation with the extent of reduction in the fibrillation by molecular entities determined using Thioflavin T and 8-anilinonaphthalene sulfonate-based fluorescence assays. Isothermal Titration Calorimetry has permitted understanding nature of interaction of potential inhibitors with the protein at different fibrillation stages in terms of standard molar enthalpy of interaction whereas Differential Scanning Calorimetry has enabled understanding extent of reduction in thermal stability of protein at these stages. The approach adopted here highlights physical chemistry underlying such biologically important processes and hence has significance in deriving guidelines for rational drug design.

# AWARD LECTURES



*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# OUR CONTRIBUTIONS TO CHEMICAL ENGINEERING THERMODYNAMICS

**M.S. ANANTH**

Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai-600036, India
e-mail: msa1945@gmail.com

We developed a perturbation theory for calculating the effect of orientation-dependent intermolecular forces on the thermodynamic properties of molecular fluids. This work was one of the earliest studies of its kind in engineering (Molecular Physics 1973 and 1974). The Self-Consistent Local Composition (SCLC) model for thermodynamic properties of non-electrolyte solutions. The model incorporates correct pair counting, the effect of the nearest as well as the second nearest neighbor interactions and uses temperature-independent interaction parameters. The theory correlates VLE data as well as the UNIQUAC model. Recently, we published a paper in a special issue of Langmuir in honour of Prof. Keith Gubbins. In this work (Langmuir, 33(42), 2017) the Gibbs-Tolman model is augmented to take into account the effect of the density gradient in the transition zone. The augmented model is shown to fit the data for 152 pure liquids and 57 liquid mixtures with absolute average deviations of 2 % and 3 % respectively.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

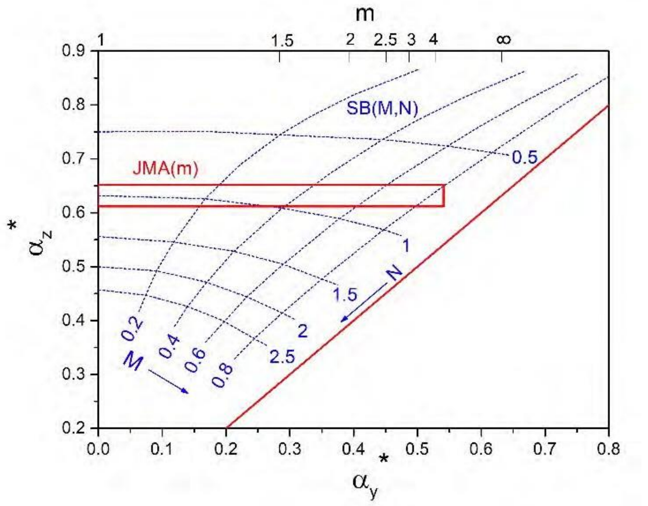
# Universality of Master Plots in Thermal Analysis

**JIŘÍ MÁLEK**[1]*

[1]Department of Physical Chemistry, Faculty of Chemical Technology,
University of Pardubice, Studentská 573, 532 10 Pardubice, Czech Republic
*Corresponding author: e-mail: jiri.malek@upce.cz

**Keywords**: kinetic analysis, DTA, DSC, TG, master plots

The master plots can be easily obtained from isothermal or nonisothermal experiments. Their comparison with the theoretical prediction for kinetic models can be very helpful for selection of the type od appropriate description of thermal analysis kinetic data. Historical overview from methods described by Sharp et al. [1] to YZ-master plots [2-4], and Ozawa's generalized time concept [5-8] is provided and thoroughly discussed. It is shown how these methods can succesfully be used to analyze complex and competitive kinetic processes in a large variety of materials.



**References**

[1] J.H. Sharp, G.W. Brindley, B.N.N. Achar, *J. Am. Ceram. Soc*. 49 (**1966**) 379.
[2] J.M. Criado, J. Málek and A. Ortega, *Thermochim Acta*, 147 (**1989**) 377.
[3] J. Málek, *Thermochim Acta*, 200 (**1992)** 257.
[4] J. Málek, T. Mitsuhashi and J.M. Criado, *J. Mater. Res.*, 16 (**2001)** 1862.
[5] T. Ozawa, *Bull. Chem. Soc. Jpn.* 38 (**1965**) 1881.
[6] T. Ozawa, *J. Therm. Anal*., 100 (**1986**) 109.
[7] F.J. Gotor, J.M. Criado, J. Málek and N. Koga, *J. Phys. Chem. A*, 104 (**2000**) 10777.
[8] J. Málek, N. Koga, L.A. Pérez-Maqueda and J.M. Criado, *J. Therm. Anal. Calorim.*, 113 (**2013)** 1437.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# The effects of natural environmental storage on the aging rate and thermal hazard characteristics of firecrackers

Chu-Yuan Yang[1], Wei-Chun Chen[2, *], Chi-Min Shu[1,3,*]
[1]Department of Safety, Health, and Environmental Engineering, YunTech, 123, University Rd., Sec. 3, Douliou 64002, Yunlin, Taiwan, ROC
[2]Bachelor Program in Industrial Technology, YunTech, 123, University Rd., Sec. 3, Douliou 64002, Yunlin, Taiwan, ROC
[3] Department and Graduate School of Safety, Health, and Environmental Engineering, YunTech., 123, University Rd., Sec. 3, Douliou, Yunlin, 64002, Taiwan, ROC
*Corresponding author: e-mail: chenwchun@gemail.yuntech.edu.tw and shucm@yuntech.edu.tw

**Keywords**: Explosion-like fireworks, aging phenomenon, simultaneous thermogravimetric analyzer, apparent activation energy, thermal stability

This study will provide an in-depth understanding of the impact of explosion-like fireworks on the hazardous properties of gunpowder compared with traditional firecrackers and environmentally friendly firecrackers stored in a normal room temperature environment for years and aging, using field emission scanning electron microscope (FE-SEM) and X-Ray photoelectron spectroscopy (XPS) observe the signs of aging caused by the influence of storage time on the sample microstructure and elements, it can be seen from the microscopic surface that firecrackers that have been stored for a long time have cracks and oxides due to oxidation and aging., then use simultaneous thermogravimetric analysis (STA) and advanced thermal analysis software to obtain thermal hazard parameters and calculate apparent activation energy. The difference in mass loss of traditional firecrackers in STA between 2005 and 2022 is significant, with a difference of 9.876%. The difference in quality loss of environmentally friendly firecrackers between 2012 and 2022 is less obvious, the difference is only 1.115%, showing that the aging of traditional firecrackers reduces thermal stability more seriously.

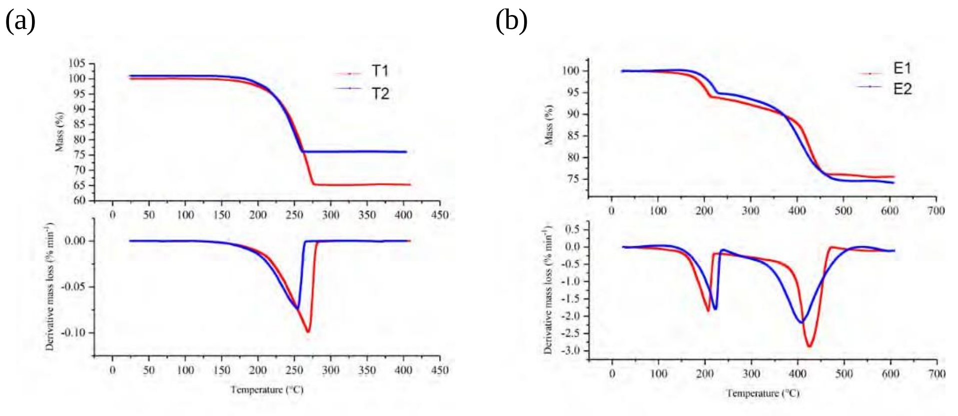


Fig. 1: The results of TG and DTG (a) traditional firecrackers; (b) environmentally friendly firecrackers

# Design and construction of a refrigerator-cooled adiabatic calorimeter for heat capacity measurement in liquid helium temperature region

**Ji-Peng Luo[1], Nan Yin[1], Jia-Bao Lu[1], Zhi-Cheng Tan[1], Quan Shi[1]***

[1]Thermochemistry Laboratory, Dalian Institute of Chemical Physics, Chinese Academy of Sciences,
Dalian 116023, P.R. China
*Corresponding author: e-mail: shiquan@dicp.ac.cn

**Keywords**: adiabatic calorimeter, low-temperature, heat capacity, refrigerator

Heat capacity is a fundamental thermodynamic property of a substance. Although heat capacity values and related thermodynamic functions are available for many materials, low-temperature heat capacity measurements, especially for novel materials, can still provide valuable insights for research in physics, chemistry, thermodynamics, and other fields. Reliable low-temperature heat capacity data are typically measured using classical adiabatic calorimeters, which use liquid helium as the refrigerant to provide a cryogenic environment for heat capacity measurements. However, liquid helium is not only expensive but also not easy to obtain, which greatly limits the application of adiabatic calorimetry.

In this work, an accurate adiabatic calorimeter equipped with a Gifford–MacMahon refrigerator was designed and constructed for measuring the heat capacity of condensed matter in the temperature range from 4 to 100 K. The Gifford–MacMahon refrigerator was utilized to provide a stable liquid helium-free cryogenic environment. A simple mechanical thermal switch assembly was designed to facilitate switching between refrigeration mode and adiabatic measurement mode of the calorimeter. Based on the measurement results of standard reference materials, the optimized repeatability and accuracy of heat capacity measurements were determined to be within 0.8% and 1.5%, respectively. Furthermore, this adiabatic calorimeter only requires electricity to operate in the liquid helium temperature range, which may significantly advance the research on low-temperature heat capacity based on adiabatic calorimetry.

**References**
[1] J. P. Luo, N. Yin, J. B. Lu, Z. C. Tan, and Q. Shi, *Review of Scientific Instruments*, 95 (**2024**) 035114.
[2] P. F. Rosen and B. F. Woodfield, *Journal of Chemical Thermodynamics*, 141 (**2020**) 105974.
[3] H. Hikawa, M. Oguni, and H. Suga, *Journal of Non-crystalline Solids*, 101 (**1988**) 90.
[4] I. Catarino and G. Bonfait, *Cryogenics*, 40 (**2000**) 425.
[5] E. Nishiyama, I. Tsukushi, J. Fujimura, and M. Yokota, *Thermochimica Acta*, 692, (**2020**) 178751.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermal analysis and calorimetry as tools for assessing the properties of different oil shales and their conversion products

**BIRGIT METS***

Department of Chemistry and Biotechnology, Tallinn University of Technology, Ehitajate tee 5,
Tallinn, Estonia
*Corresponding author e-mail: birgit.mets@taltech.ee

**Keywords**: thermal analysis, DSC, fossil fuel valorization, mineral resources

The characterization of fuels usually includes using numerous analytical techniques. Thermal analysis and calorimetry have proven to be extremely useful tools for obtaining different parameters, such as the heating value, the amount of organic matter or carbonate minerals, or something as simple as measuring the ash content, obtaining several parameters at once with minimal sample preparation.

A good example of this is the use of measurement data of thermogravimetric analysis to simulate industrial processes or to obtain kinetic parameters. Oxy-fuel combustion analysis showed that substituting nitrogen with $CO_2$ enabled separating the decomposition of carbonate minerals – dolomite exhibited a lower temperature than calcite, which under regular combustion conditions occurred as one single step. [1] Another use is the calculation of kinetic parameters, which enables assessing the conversion of organic matter, thereby decreasing the need for industrial testing. [2] Technological developments have also awarded us the opportunity to use high-speed furnaces to simulate the thermal behaviour of particles in industrial conditions. [3]

Oil shale organic matter exhibits vast opportunities for valorisation due to its polymeric structure and richness in functional groups – it is an aliphatic branched macromolecule cross-linked with aromatic (phenolic) units and differently bonded oxygen atoms in various ratios. Oil shale treated with air and nitric acid generates oxidation products consisting of different chain length dicarboxylic acids (DCAs). Pure DCAs show a zig-zag effect – even number of carbon atoms yield higher melting points than the next odd-numbered DCAs, meaning acids with an even number of C atoms require higher decarboxylation temperatures. For oil shales from Estonia, Syria, Brazil, Jordan and the USA the DCA production was shown not to depend on the amount of organic matter (varied from 14 to 40%). Thermal analysis and calorimetry were used to characterize the obtained mixtures.

## References

[1] Loo, L.; Maaten, B.; Siirde, A.; Pihu, T.; Konist, A., *Fuel Processing Technology*, 134 (**2015**) 317.

[2] Maaten, B.; Loo, L.; Konist, A.; Pihu, T.; Siirde, A., *Journal of Analytical and Applied Pyrolysis*, 128 (**2017**) 405.

[3] Maaten, B.; Siirde, A.; Vahur, S.; Kirsimäe, K., *Journal of Thermal Analysis and Calorimetry*, 148 (**2023**) 1647.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Calcium Silicate Hydrates with Intercalated Transition Metal Ions: Preparation Techniques, Thermal Properties, and Applications

**T. DAMBRAUSKAS[1]*, K. BALTAKYS[1]**

[1]Department of Silicate Technology, Kaunas University of Technology, Radvilenu pl. 19, LT-50270, Kaunas, Lithuania
*Corresponding author: e-mail: tadas.dambrauskas@ktu.lt

**Keywords**: thermal analysis, calcium silicate hydrates, catalytic activity, hydrothermal synthesis

Calcium silicate hydrates play an important role in the sustainability because they are the main compounds in the cement chemistry and they are used as heat insulating materials, as adsorbents for $CO_2$ or contaminants from water, environmentally friendly cementitious materials, etc. [1-2]. Calcium silicate hydrates are a group of inorganic compounds which include more than 40 synthetic and natural minerals, with various compositions in a wide range of $CaO/SiO_2$ ratio between 0.44–3.0. Although these compounds have been known for more than century and lots of research on them was performed, their chemistry is still not fully understood [1, 3-4]. An even more complicated area is understanding the influence of transition metal ions on the formation and properties of calcium silicate hydrates [5]. The complexity of the research is determined not only by the large number of ions that can intercalate into the structure of calcium silicate hydrate, but also by different uptake capacity of calcium silicate hydrates for foreign ions under different synthesis conditions (duration, temperature, water to solid ratio, mixing intensity, etc.) [5-6]. In addition, transition metal ions can be intercalated into the structure of these compounds by both synthesis and adsorption methods.

Understanding both the formation and thermal properties of calcium silicate hydrates with intercalated transition metal ions can lead to a better understanding of cement chemistry and predict their potential use in sustainability.

In this lecture the influence of transitions metal ions ($Co^{2+}$, $Cu^{2+}$, $Fe^{3+}$, and $Cr^{3+}$ ions) on thermal properties of higher basicity calcium silicate hydrates, obtained under different techniques, will be discussed. The obtained results were confirmed by numerous advance thermal analysis techniques: In-situ X-ray diffraction, different scanning calorimetry, simultaneous thermal analysis, dilatometry, microcalorimetry, etc.

**References**

[1] I.G. Richardson, Ian G. Cem. Concr. Res., 38 (2008) 137–158.
[2] K. Baltakys and T. Dambrauskas. *Synthetic Gyrolite: Dual Solution for Wastewater Treatment and Portland Cemen*t. Cham: Springer Nature Switzerland, 2024.
[3] Y. Yan, et al. Cem. Concr. Res., 172 (2023) 107250.
[4] X. Wang, et al. Mater. Sci. Eng. B., 299 (2024) 116930.
[5] X. Liu, et al. Constr. Build, Mater., 413 (2024) 134931.
[6] H. Tian, et al. Constr. Build, Mater., 301 (2021) 124071.

# Influence of chemical composition and structure on the cooperative fluctuation in supercooled glass-forming liquids

**K. HALLAVANT[1]*, M. MEJRES[1], J.E.K. SCHAWE[2], A. ESPOSITO[1], A. SAITER-FOURCIN[1]**

[1]University Rouen Normandy, INSA Rouen Normandy, CNRS, 76000 Rouen, France
[2]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland.
*Corresponding author: e-mail: kylian.hallavant@univ-rouen.fr

**Keywords**: Thermal analysis, FSC, DSC, TOPEM, Glass transition, Organic polymers, Selenium

The kinetics of the glass transition and the characteristic size of the fluctuating spatio-temporal domains in supercooled glass-forming liquids, i.e., the Cooperatively Rearranging Regions (CRR), were measured upon cooling over a broad range of cooling rates using Differential Scanning Calorimetry (DSC), stochastically temperature modulated DSC (TOPEM) and chip-based Fast Scanning Calorimetry (FSC), through the approach of Donth [1]. The investigations were conducted on a selection of fragile glass formers (fragility indices between 80 and 140), with a large variance in the atomic or molecular structure but comparable thermal glass transition temperatures $T_g$, with the aim of evaluating the influence of chemical composition and structure on the CRR size and the associated temperature fluctuation. The selected materials are two polymers (poly(vinyl acetate) (PVAc), poly(lactic acid) (PLA)) as well as a chalcogenide glass-former (selenium). It appears that the CRR size plotted against the reduced temperature $T/T_g$ follows the same trend, irrespective of the considered glass-former [2].

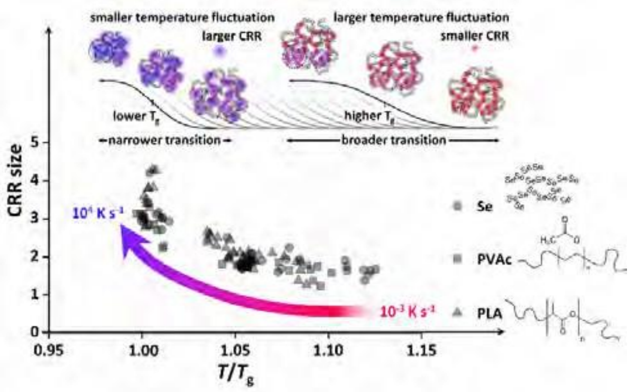


Fig. 1: Evolution of the CRR size against the reduced temperature $T/T_g$

**References**

[1] E. Donth, The Size of Cooperatively Rearranging Regions at the Glass Transition, *J. Non-Cryst. Solids* (**1982**), 53 (3), 325–330.

[2] K. Hallavant, M. Mejres, J.E.K Schawe, A. Esposito and A. Saiter-Fourcin, *J. Phys. Chem. Lett,* (**2024**), 4508-4514.

**ICTAC TG AL 03**

# Thermal Dehydration Kinetics of Copper(II) Sulfate Pentahydrate across Different Water Vapor Pressures

**MITO HOTTA, NOBUYOSHI KOGA***

Grad. Sch. Humanities and Social Sciences, Hiroshima Univ., Higashi-Hiroshima 739-8524, Japan
*Corresponding author: e-mail: nkoga@hiroshima-u.ac.jp

**Keywords**: thermal dehydration, $CuSO_4·5H_2O$, Kinetics, water vapor pressure

The kinetics of the thermal dehydration of inorganic hydrates is generally affected by atmospheric and self-generated water vapor. Copper(II) sulfate pentahydrate ($CuSO_4·5H_2O$, CSPH) that proceeds in three-step thermal dehydration to form anhydride via trihydrate and monohydrate is such an example. The effect of atmospheric water vapor on the first reaction step of the thermal dehydration of CSPH exhibits complex behavior known as the Smith–Topley effect [1].

Recently, the authors established an extended kinetic approach to the reversible thermal dehydration based on Eq. (1) [2–4]:

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = A\exp\left(-\frac{E_\mathrm{a}}{RT}\right) f(\alpha)\, h\left(p(\mathrm{H_2O}), P_\mathrm{eq}(T)\right)$$

$$\text{with} \quad h\left(p(\mathrm{H_2O}), P_\mathrm{eq}(T)\right) = \left(\frac{1}{p(\mathrm{H_2O})}\right)^a \left[1 - \left(\frac{p(\mathrm{H_2O})}{P_\mathrm{eq}(T)}\right)^b\right], \qquad (1)$$

where $A$ and $E_a$ are the Arrhenius preexponential factor and apparent activation energy, respectively. With aid of the accommodation function (AF; $h(p(H_2O), P_{eq}(T))$), the reversible thermal dehydration of inorganic hydrates was universally described as a function of temperature ($T$), degree of reaction ($\alpha$), and water vapor pressure ($p(H_2O)$) with reference to the equilibrium water vapor pressure of the reaction ($P_{eq}(T)$).

In this study, the kinetics of the individual reaction steps of the thermal dehydration of CSPH was systematically investigated under various heating and $p(H_2O)$ conditions using a humidity-controlled thermogravimetry (HUM-TG, Rigaku). The kinetic data for individual reaction steps recorded under isothermal and linear nonisothermal conditions at four selected $p(H_2O)$ values were universally analyzed using the extended kinetic equation (Eq. (1)) through parameterizing the effect of water vapor by the exponents in the AF, i.e., ($a$, $b$), and determining the universal Arrhenius parameters, i.e., ($E_a$, $A$), of the individual reaction steps. The possible causes of the Smith–Topley effect are discussed based on the results of the extended kinetic approach.

**References**
[1] M. L. Smith, B. Topley, *Proc. Royal Soc.*, 134 (**1931**) 224–245.
[2] N. Koga, L. Favergeon, S. Kodani, *Phys. Chem. Chem. Phys.*, 21 (**2019**) 11615–11632.
[3] Y. Yamamoto, L. Favergeon, N. Koga, *J. Phys. Chem. C*, 124 (**2020**) 11960–11976.
[4] M. Hotta, N. Koga, *Thermochim. Acta*, 733 (**2024**) 179699.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Calorimetric and thermodynamic analysis of cowpea β-vignin: unveiling effects of seed germination on the conformation of a storage protein

**FRANCESCA SAITTA*, STEFANO DE BENEDETTI, ALESSIO SCARAFONI, DIMITRIOS FESSAS**

Department of Food, Environmental and Nutritional Sciences (DeFENS), Università degli Studi di Milano, Via Celoria 2, 20133, Milan, Italy
*Corresponding author: e-mail: francesca.saitta@unimi.it

**Keywords**: thermal denaturation, storage protein, DSC, thermodynamics, germination

Storage proteins have been generally considered as a mere nitrogen reserve that supports seedling growth during germination [1]. Nevertheless, new findings indicate that several biological activities become manifest because of the action of intermediate polypeptide fragments that are formed upon a selective breakdown of specific peptide bonds occurring through a regulated mechanism [2].

β-vignin is the most represented storage protein in cowpea seeds (*Vigna unguiculata*, L. Walp) and belongs to the vicilin-like family [3]. It is synthesized during seed development and consists of two main differently glycosylated isoforms. Moreover, it exists in a monomer-to-trimer equilibrium that depends on the environment pH: the higher the pH, the greater the trimer-to-monomer ratio [4].

Up to now, cowpea β-vignin molecular properties have been object of few studies, and many aspects have not been addressed yet. The full understanding of cowpea β-vignin structural and physicochemical properties is crucial to disclose possible biological roles and to approach applicative uses in various fields, including eco-friendly plant defense, nutrition and nutraceutics.

In this frame, the present work was aimed at gaining insights on the thermodynamic stability of both the cowpea native β-vignin and the structures produced during seed germination. Therefore, purified β-vignin was subjected to a limited proteolysis by using cowpea proteases extracted from germinating seeds to simulate the early germination process, and a calorimetric investigation was performed through high-sensitivity DSC on both the undigested and digested β-vignin in different buffered environments (pH 9.0, 8.5 and 6.5). A thermodynamic analysis was also accomplished on the β-vignin undigested form to assess the protein stability and thermal denaturation mechanism. The results revealed that the storage protein behaviour is rather peculiar if compared to proteins with other biological functions.

**References**

[1] Y. Wakasa, F. Takaiwa, in *Brenner's Encyclopedia of Genetics*, 2nd ed. Academic Press, San Diego, CA, USA, 2013.
[2] J.P. Marcus, J.L. Green, *et al.*, *Plant J. Cell Mol. Biol.*, 19 (**1999**) 699.
[3] R.L. Freitas, A.R. Teixeira, R.B. Ferreira, *J. Agric. Food Chem.*, 52 (**2004**) 1682.
[4] S. De Benedetti, C. Leogrande, *et al.*, *Molecules*, 27 (**2022**) 277.

# Emerging Prospective of Role of Solvents: towards Dissolution of Biomolecules

**Dharmendra Singh***

Institute of Engineering & Technology, Dr. Rammanohar Lohia Avadh University Ayodhya U.P.-224001, India
*Corresponding author: e-mail: singh2017chem@gmail.com

The disintegration of biomolecules into its simpler molecules has been a long term research topic to enhance their applicability as new therapeutic agents for treating various diseases and understand their complex structures [1]. For preceding such process, we need an adequate media for dissolution as well as stabilization. In search of better alternative of organic solvents, Ionic liquids (ILs) are found to be very promising. ILs are molten salts which has several distinguished features so it can able to replace the volatile organic solvents[2]. In this framework, we developed 1,2,4-triazolium-based highly polar organic solvents, which are found to be good agreement for the stabilization of ascorbic acid and heme protein through thermophysical and photophysical studies [3-4]. Moreover, effect of concentration and anion of ILs on the stabilization of digestive enzymes (pepsin) has been studied through numerous photophysical studies and found that lower concentration of imidazolium-based ILs are more promising for structural activity and functionality of enzymes [5]. Additionally, performing biocatalysis in nonaqueous solvents is advantageous as it imparts enhanced solubility to hydrophobic substrates and an ability to increase the temperature for shifting reaction equilibrium in the forward direction. Thus, at IIT Bombay, we developed α-chymotrypsin-polymer-ILs based composites, which are applicable for biocatalytic reactions as non-aqueous media [6]. Moreover, our results, therefore, show the stabilization of enzymes/proteins in a neat as well as aqueous IL environment to yield a composite liquid, which not only acts as a non-volatile and environmentally benign solvent, but also provides a biocatalytic platform capable of carrying out reactions relevant for biotransformations, food processing, drug delivery, and various other applications.

## Reference

[1] M. Sivapragasam, M. Moniruzzaman and M. Goto, *Biotechnol. J.*, 11 (**2016**) 1000–1013.
[2] D.Singh, G. Sharma and R. L. Gardas, *J. Phys. Chem. B,* 120 (**2016**) 4834– 4842.
[3] D. Singh, G. Sharma and R.L. Gardas, *J. Mol. Liq.*, 244 (**2017**) 55–64.
[4] D. Singh, S. K. Panigrahi, G. Sharma, and R. L. Gardas, *J. Mol. Liq*., 349 (**2022**) 118213.
[5] P. Singh, O.P. Verma, N. Dey and D.Singh, *J. Mol. Liq*., 391B (**2023**) 123366.
[6] A. Mukhopadhayay, D. Singh, and K. P. Sharma, *Biomacromolecules,* 21 (**2020**) 867–877.

# Unravelling Thermodynamics Signatures Accompanying Binding of Protein to Lipid Nanoparticles: A Spectroscopic and Calorimetric Analysis

**JYOTI RATHEE[1], NAND KISHORE[1*]**

[1]Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai, India
*Corresponding author e-mail: nandk@chem.iitb.ac.in

**Keywords**: Thermal Analysis, Calorimetry, BSA, Spectroscopy

With the booming development of nano-medicines, significant attention has been paid to biocompatible solid lipid nanoparticles (SLNs) owing to their desired nano-assembly properties such as long-term stability, longer circulation time, higher drug loading, and encapsulation efficiency [1]. When the lipid nanoparticles are administrated in in-vivo, their bio-distribution, metabolism, and cellular internalization are significantly affected by the diversified biological fluids having different pH and abundant biomolecules (amino acids and peptides) [3-5]. Therefore, the study of the binding interactions of the SLNs with the serum albumins will pave the way to understanding the bimolecular recognition process essential for the rational drug design process. The current investigation delineates the quantitative analysis of the thermodynamic signatures associated with the interactions of Bovine Serum Albumin (BSA) with lipid nanoparticles using a combination of calorimetric and spectroscopic techniques. The particle size of the prepared SLNs is (100 ± 3) nm which after incubation with SLNs increases to (102±5) nm. The energetics of the interactions of the BSA with the lipid nanoparticles were examined using fluorescence and isothermal calorimetry. The thermodynamic parameters accompanying the interactions (($\Delta \mathrm{H}m$ 0 ) = + (9.8 ± 0.2) kJ/mol and $\Delta Sm$ 0 = +(13.96± 3.0) kJ/mol) suggest the association is hydrophobic. The interactions between the hydrophobic part of the lipid nanoparticles and hydrophobic patches of the BSA molecule are indicated. SLNs showed binding affinity of the order of 102 which suggests the weak interactions accompanied by the blue shift in the fluorescence spectra. UV-visible spectra also confirmed the change in the microenvironment of the tryptophan towards a more nonpolar environment with an affinity of the order of 103 . Differential scanning calorimetry results suggest the stabilization of the BSA in the presence of the SLNs. Further, CD spectroscopic signatures reveal a small increase in the α-helicity of the secondary structure, while the tertiary structure of protein is maintained. Overall, obtained results demonstrated significantly good affinity of SLNs with BSA, facilitating their easy transportation to desired targeted sites.

### References

[1] H. Moss, P. Popova, S.R. Hadrup, K. Astakhova, M. Taskova, *Mol. Pharm.*, 16 (**2019**) 2265–2277.
[2] W. Wang, Z. Huang, Y. Li, W. Wang, J. Shi, F. Fu, Y. Huang, X. Pan, C. Wu, *Acta Pharm. Sin. B.*, 11 (**2021**) 1030–1046
[3] S. Das, W.K. Ng, R.B.H. Tan, *Eur. J. Pharm. Sci.* 47 (**2012**) 139–151.
[4] J. Wolfram, Y. Yang, J. Shen, A. Moten, C. Chen, H. Shen, M. Ferrari, Y. Zhao,124 (**2014**) 17–24.
[5] P. Del Pino, B. Pelaz, Q. Zhang, P. Maffre, G.U. Nienhaus, W.J. Parak, *Mater. Horizons*. 1 (**2014**) 301-313

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Study of Molecular Interactions for the Supramolecules in Aqueous, Aqueous–Drug and Aqueous–KBr Solutions at 298.15 K

**VASIM R. SHAIKH**

School of Chemical Sciences, K. C. E. Society's Moolji Jaitha College (Autonomous),
Jalgaon-425001, Maharashtra, India.
*Corresponding author: vasimshaikh84@gmail.com

**Keywords**: osmotic coefficient, activity coefficient, transfer Gibbs free energies, equilibrium constant, pair and triplet interaction parameters.

The osmotic coefficient measurements have been carried out for ternary aqueous solutions containing a fixed concentration of α–Cyclodextrin (α–CD) and 2,2,2–Cryptand of ~ 0.1 $mol \cdot kg^{-1}$ and varying the concentrations (~0.012 to ~0.21 $mol \cdot kg^{-1}$) of drugs procaine hydrochloride (PC·HCl), Lidocaine hydrochloride (LC·HCl), Tetracaine hydrochloride (TC·HCl), Ranitidine hydrochloride (RT·HCl) and KBr at 298.15 K using vapour pressure osmometry for understanding the complexation phenomenon between α–CD and drugs and 2,2,2-Cryptand and KBr. The water activities for each ternary system were measured and used to obtain the activity coefficients of α–CD or 2,2,2–Cryptand and drugs or KBr. The transfer Gibbs free energies have been calculated using the activity data. These were further used for the estimation of pair and triplet interaction parameters. By applying the method based on the application of the McMillan–Mayer theory of virial coefficients to transfer free energy data, the salting constant and thermodynamic equilibrium constant values have been estimated at 298.15 K. All these results are presented and explained in light of host–guest interaction concepts.

**References**
[1] W. Saenger, *Angew. Chem. Int. Ed.* 17 (**1978**) 694.
[2. D. J. Cram, *Angew. Chem. Int. Ed.* 27 (**1988**) 1009.
[3] J. M. Lehn, *Angew. Chem. Int. Ed.* 27 (1**988**) 89.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

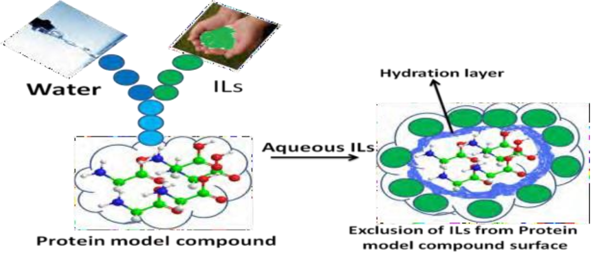
# “Thermodynamic characterization of Structural Basis for the Enhanced Solubility, Stability of Protein Model Compounds and Peptide Backbone Unit in Ammonium based Ionic Liquids”

**T. VASANTHA**

Department of Chemistry, Sri Venkateswara College, University of Delhi,
Dhaula Kuan, New Delhi-110021, India.
Author: e-mail: vasanthathoti@gmail.com, tvasantha@svc.ac.in

**Keywords**: Ionic Liquids, Amino acids, Solubility, Transfer free energy, Biocompatibility.

Protein folding/unfolding is a fascinating study in the presence of co-solvents, which protect/disrupt the native structure of protein, respectively. Ionic liquids (ILs) are finding a vast array of applications as novel co-solvents for a wide variety of biochemical processes that include protein folding. The solubility measurements, as a function of IL concentration at 25 °C have been exploited to quantify and interpret biomolecular interactions between model compounds of glycine peptides (GPs) and Amino Acids (AAs) with ammonium based ILs. The different investigated aqueous systems consist of zwitterionic peptides: glycine (Gly), diglycine ($Gly_2$), triglycine ($Gly_3$), tetraglycine ($Gly_4$) cyclic glycylglycine (c(GG)), in the presence of six ILs such as diethylammonium acetate, diethylammonium hydrogen sulfate, triethylammonium acetate, triethylammonium hydrogen sulfate, triethylammonium dihydrogen phosphate and trimethylammonium acetate.

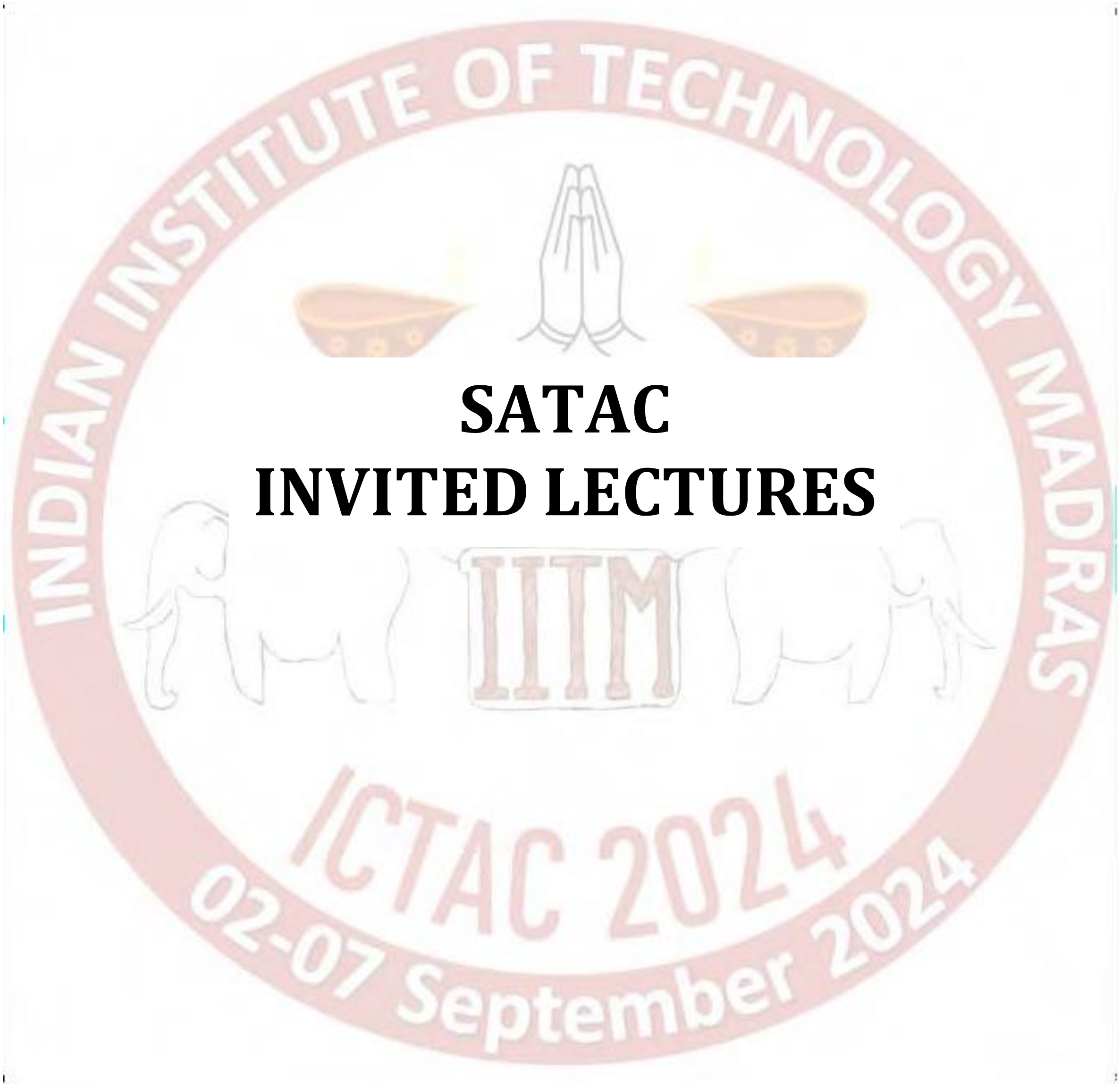


**Scheme1. Representation of Model Compounds in the Presence of ILs**

We have observed positive values of $\Delta G'_{tr}$ for GPs from water to ILs, indicating that interactions between ILs and GPs are unfavorable, which leads to stabilization of the structure of model protein compounds. Our results show the decrease in the aqueous solubility (salting-out) of the AA with increasing the concentration of ILs indicate towards the unfavorable interaction of the ILs with the AA surface. These results explicitly elucidate that all alkyl ammonium ILs act as stabilizers for the compounds through the exclusion of ILs from model compounds of proteins and also reflects the effect of alkyl chain on the stability of protein model compounds.

## References

1. T. Vasantha, T. Kavitha, Awanish Kumar, P. Venkatesu, R.S. Rama Devi. *J.Mol.Liq*. **2015**, *208*,130-136.
2. T. Vasantha, P. Attri, P. Venkatesu, R.S. Rama Devi. *J.Chem. Thermodyn*, **2013**, *56*, 21.



# SATAC
# INVITED LECTURES

**SATAC IL 01**

# Hydration of Blended cement in presence of nanomaterials

**N. B. SINGH**
Department of Chemistry and Biochemistry and Research and Development Cell
Sharda University, Greater Noida, UP, India
Corresponding author: email: n.b.singh@sharda.ac.in

**Keywords**: Blended cement, Heat Evolution, Nanomaterials, nano CuO, Compressive strength

The escalating environmental concerns associated with traditional Portland cement production, primarily due to its high carbon dioxide emissions (0.73-0.85 tons of $CO_2$ per ton of OPC) [1], have intensified the search for more sustainable construction materials. Low-carbon cement-based materials are highly desirable for sustainable construction because they reduce energy consumption and greenhouse gas emissions [2]. The replacement of Portland cement with supplementary cementitious materials (SCMs) to produce blended cement has become a standard practice. Among various SCMs, Fly ash (FA) and granulated blast furnace slag (GBFS) are most important [3]. The use of these materials in cement-based materials significantly reduces carbon emissions [4], decreases the consumption of natural mineral resources and energy, and lowers production costs. Thus, incorporating GBFS in cement aligns with the goals of carbon neutrality and sustainable development [4]. Heat of hydration, Thermal methods, X-ray diffraction and Scanning electron microscopic studies have been used to study and understand the hydration process of blended cements in presence of different nanomaterials. A Symbolic heat evolution profile in presence of nano CuO is given in Fig. 1.

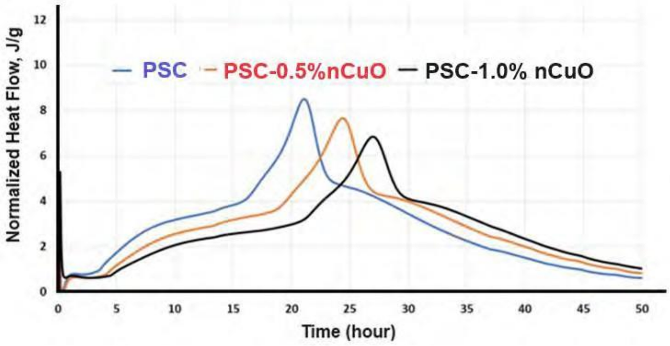


Fig. 1: Normalised heat release curve of PSC with nCuO

Different techniques have been used and the effect of nanomaterials on the hydration of blended cement has been discussed in detail.

**Keywords**: Blended cement, Heat Evolution, Nanomaterials, nano CuO, Compressive strength

## References

[1] Zhijun He , Xiaodong Zhu , Junjie Wang, Mulan Mu , Yuli Wang,. Construction and Building Materials, 211(**2019**)965-973
[2] Xi Liu, Pengkun Hou, Heng Chen, , Construction and Building Materials 282(**2021**)122705
[3] A. Bougara, C. Lynsdale, N.B. Milestone, , Constr. Build. Mater. 187 (**2018**) 339–347
[4] Zhenhai Xu, Zhaoheng Guo, Yasong Zhao , Shujun Li, Xu Luo, Gaofeng Chen, Cheng Liu, Jianming Gao, Journal of Building Engineering 64 (**2023**) 105657

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Reactivity and Thermo–Magnetic Spin Glass transition of Nano-Ferrites by Thermal Analysis and Calorimetry

**N. S. Gajbhiye ***

Indian Institute of Technology, Kanpur
*Corresponding author: e-mail: gajbhiyens@gmail.com

Reactivity study of metallo-organic complexes (the precursors) for the nanoparticles formation was planned for the magnetic soft and hard ferrites such as: spinel ferrites (MFe2O4 where M = Fe, Ni, Co, Mn), hexagonal ferrites (MFe12O19 where M = Ba, Sr, Pb) and rare-earth iron garnets (R3Fe5O12 where R = Sm, Tb, Dy, Ho, Er, Yb). Thermal decomposion of precursor is a multi – step process and is studied by using thermal techniques –TG / DTA / DSC with EGA. The typical kinetic parameters like activation energy (Ea) and frequency factor (A) by using Coats-Redfern method were calculated for the formation of ferrites nanoparticles. The isolation of the intermediate steps and characterization were done by using XRD, IR, NMR and AAS techniques. Thermal techniques TG/DTG/DSC were utilized to control the particle size, morphology, stoichiometry and investigated for phase transitions - spin - glass transition of the ferrite materials. An irreversible redistribution of cations occurred in MnFe2O4 ferrite lattice at 673 K. Also, 'Hopkinson effect' was rediscovered in soft ferrites. Thermo-magnetic measurements on ferrites exhibit spin canting structure at the surface of the nanoparticles. Further, the spin glass behavior was studied in detail for MnFe2O4 nanoparticles by using Thermal Analysis and Calorimetry techniques. The magnetic spin glass transition temperatures, Tb - Blocking Temperature and Tf - Spin freezing temperature, were are measured by the magnetic field dependent, ZFC / FC, studies and were extensively explored using low temperature Calorimetry.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Crystallization Kinetics of Multi-component Metallic Glasses using Differential Scanning Calorimetry

**Arun Pratap***

Condensed Matter Physics Laboratory, Applied Physics Department, Faculty of Technology &amp;
Engineering, The Maharaja Sayajirao University of Baroda, Vadodara -390 001, Gujarat
*Corresponding author: e-mail: apratapmsu@yahoo.com

Amorphous metallic alloys possess some unique exotic properties. They possess very high corrosion resistance due to absence of grain boundaries. They also have very high mechanical strength. Among the metallic systems, alloys with many components have higher probability of forming amorphous systems. Mixing more number of components with varying sizes lead to ‘frustration’ due to increase in the number of components avoiding crystallization. When such multicomponent amorphous alloys are subjected to heat, they crystallize in multiple steps leading to more than one exothermic peak in DSC. Many a time, these peaks also overlap each other at particular temperature. They need to be separated by increasing the resolution of DSC measuring these events. This led to the recent advancement in the instrument giving birth to ‘modulated’ DSC. The thermal analysis of the events taking place in DSC when these systems are subjected to heat is analyzed. Different exothermic reactions like crystallization and endothermic events e.g., glass transition will be monitored in DSC and modulated DSC. Crystallization is a combined process of nucleation and growth. Crystallization and glass transition both are kinetic phenomena as they are shifted to higher temperatures with increasing heating rate. Using the peak shift method, various kinetic parameters like activation energy and frequency factor will be evaluated. Both isokinetic and isoconversional methods will be used for this purpose.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Understanding thermooxidative stress on Indian mustard oil during heating in air and impact of turmeric doping

RANJIT K VERMA[1]*

[1]University Department of Chemistry, Magadh University, Bodh Gaya 824234, India
*Corresponding author: e-mail: profrkverma@gmail.com

**Keywords**: thermal analysis, DSC, mustard oil, thermooxidative decomposition, turmeric doping.

Edible oils are extensively used for cooking particularly vegetables in Indian cuisine. These have been in use for traditional half frying but there has been recent changes in the pattern of use in the kitchen wherein they are substituting butter fat (use of which was more prevalent in north India) for deep frying. These are used for frying, during food preparation. Many changes (oxidation, isomerisation, polymerization, hydrolysis etc) may take place in the cooking oil. Among them, mustard oil (rapeseed oil) has been very popular in north and eastern regions of India. It is also known for its stimulant, antibacterial, antifungal and antirheumatic activities. Knowing the oxidative stability of Indian mustard oil is important and in the present study, this has been measured by TG-DSC technique. Its oxidative stability has been investigated in presence and absence of turmeric. Usually, it has polyunsaturated fats, the omega-3 $\alpha$-linoleic acid [all-cis-9,12,15-octadecatrienoic acid], the omega-6 linoleic acid and saturated fats in the ranges of 21%, 6%, 15%, and 12% respectively. Pure oil has been heated under 4 different heating rates of 50, 100 , 150 & 200 C/min under $N_2$ /$O_2$ purging. The DSC for herbal (turmeric) doped mustard oil samples has been obtained up to 230 C @ 0.5, 1, 3, 5, 7 and 10 K/min. It was done in the atmosphere of air and oxygen with a flow rate of 50 ml/min. Approximation of kinetic parameters (E, A ) has been carried out. The activation energy of oil is strongly influenced by the amount of saturated fatty acid content in the oil. Isothermal induction period has been predicted under various heating rates. Marked changes have been observed in the pattern when the heating is done after doping with ball milled turmeric powder (after undertaking XRD, spectrophotometric, PL,VSM studies for looking into changes with ball milling time). Shelf life prediction has been done (oxidation induction time).

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Advanced Thermal Analysis of Ionic Liquids and Deep Eutectic Solvents for Sustainable Metal Recovery from Spent Batteries

**RAMESH L. GARDAS***

Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036, India
*Corresponding author: e-mail: gardas@iitm.ac.in

**Keywords**: thermal analysis, ionic liquids, deep eutectic solvents, metal recovery

As the world progresses towards more sustainable energy storage solutions, the recycling of spent lithium-ion and nickel-based batteries presents both significant challenges and opportunities. This invited talk will delve into innovative methods for enhancing metal recovery from spent batteries, with a focus on the role of thermal analysis in optimizing and understanding the performance of deep eutectic solvents (DESs) and ionic liquids (ILs).

Our discussion will begin with the application of pyruvic acid (PA)-based DESs for the efficient extraction of critical metals from spent LIB cathode materials. We will highlight the thermal analysis techniques used to characterize the thermal stability and phase behavior of Choline Chloride/PA DESs, which enable up to 99% extraction of cobalt (Co) and lithium (Li). The thermal properties are crucial in optimizing leaching conditions and ensuring the reusability of the DES for multiple cycles, thereby enhancing the sustainability of the recycling process.

The talk will also cover the emerging role of ionic liquids in the separation of critical metals from spent batteries. We will discuss the thermal analysis of various ionic liquids, including imidazolium-based and phosphonium-based ILs, to understand their thermal stability and solvation behavior. This analysis is pivotal for tailoring ILs to specific metal recovery applications and improving their efficiency compared to traditional solvents.

By integrating thermal analysis into the development and optimization of DESs and ILs, this talk will provide insights into how these advanced materials can be leveraged for more effective and sustainable recycling processes. The session will underscore the importance of thermal analysis in the design and application of these innovative solvents, contributing to the advancement of green technologies in the recycling industry.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Enhanced Carbon Capture Efficiency through Additive-Infused and Amine-Functionalized $SiO_2$ Nanoparticle Formulations

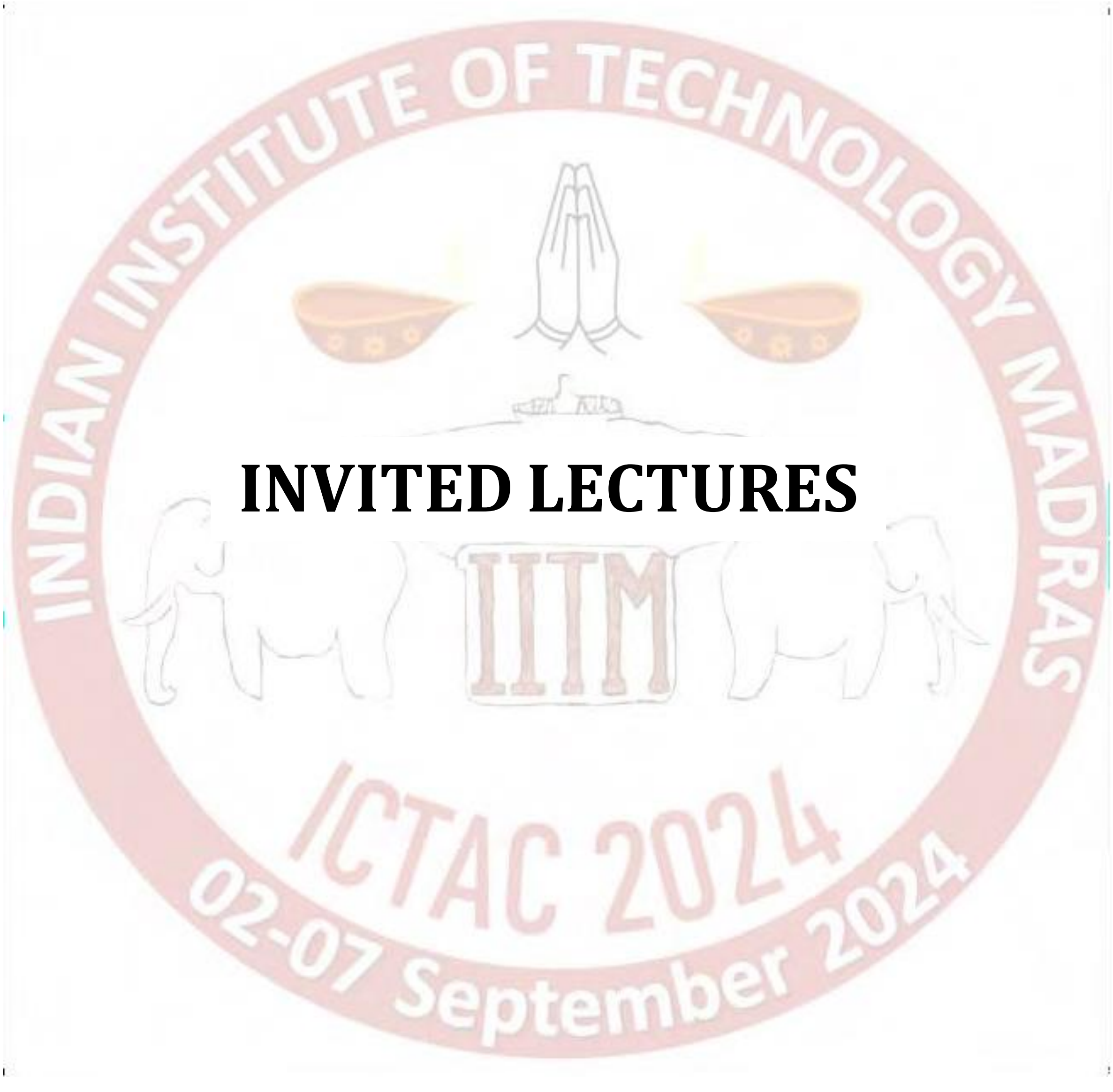
**YOGENDRA KUMAR, JITENDRA SANGWAI***

Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai-600036, India
*Corresponding author: e-mail: jitendrasangwai@iitm.ac.in

**Keywords**: absorption, carbon capture, functionalization, thermal analysis.

Capturing $CO_2$ directly from anthropogenic emissions is a critical societal responsibility, given the alarming rise in global atmospheric $CO_2$ levels. Achieving long-term negative emissions necessitates the development of techniques to extract $CO_2$ directly from the atmosphere, and industrial flue gases. Amine-based absorbent is conventionally used for carbon capture, but its utility is limited owing to high-temperature operability, energy-intensive regeneration, lower recyclability, and corrosion issues. This study utilizes a nanoformulation derived from amines, amine-functionalized nanoparticles, and other additives in an interfacial contact reactor. The experiments were carried out in an interfacial contact reactor at 298 and 320 K using DEA (30 vol.%), MEA (30 vol.%), and nanoformulations derived using DEA/MEA. Amine functionalized nanofluids are prepared using a 3-step preparation technique and characterized for stability and thermal and physical characteristics. Analysis of absorption was conducted using a 3-hour absorption process, followed by the chemical and thermal characterization of the $CO_2$-loaded and pristine solvents. Experimental observations indicate that functionalized nanofluid systems show a 15-20% increase in $CO_2$ absorption and a 10-15% improvement in capture rate. Thermal analysis of both pristine and $CO_2$-loaded solvents reveals that functionalized nanofluids exhibit greater regeneration potential than traditional DEA/MEA solvents and nearly 25-40% efficient regeneration has been observed. Additionally, the heating requirements are lower for functionalized nanofluids compared to conventional amines.

# INVITED LECTURES



*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# A Critical Appraisal of Nanofluids Research and Development

**S M SOHEL MURSHED**

IDMEC, Instituto Superior Técnico, University of Lisbon, 1049-001 Lisbon, Portugal
e-mail: smurshed@tecnico.ulisboa.pt

**Keywords**: nanofluids, thermal management, technological readiness level, challenges

The main goal of this invited talk is to provide a critical appraisal of research and development of nanofluids since its coining in the early nineties (1993-1995). Nanofluids are the suspensions of nanoscale particles in liquids such as conventional heat transfer fluids. Nanofluid is arguably one of the hot research topics in multidisciplinary fields which include thermal sciences, mechanical and materials engineering as well as nanotechnology [1-2]. Given the surge of research interests and subsequent explosion of publications it is worthy to provide such an appraisal of this new class of fluids and to critically assess their real prospects and barriers to market uptake.

The talk consists of three parts. The first part provides a critical review of the state-of-the-art research on this topic starting from its historical background to thermophysical properties results and anomalies. This part also briefly highlights how such a global surge of interest evolved and led to some chaotic and inconclusive circumstances. The second part assesses its potential particularly in thermal management systems and applications involving convective and boiling heat transfer processes. The final part of this speech discusses nanofluids' current technological readiness level, challenges, and barriers towards their real-world applications. In principle, this keynote addresses and answers the key questions: do nanofluids exabit anomalous increase in the heat transfer (conduction, convection and boiling) performances and are they capable of meeting the modern cooling demands and energy (thermal) needs?

.

**References**

[1] S.M.S. Murshed, Fundamentals and Transport Properties of Nanofluids, Royal Society of Chemistry, London, UK, 2022.
[2] S.M.S. Murshed, Nanofluids: Synthesis, Properties and Applications, Nova Science Publishers Inc., New York, 2014.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Exploring the Role of Aspartic Acid in Modulating Micellization Behavior of Cationic Cetyltrimethylammonium Bromide

**ANISH KUMAR SAH[1], ZAINEBO. ETTARHOUNI[2], AYSHA B. MEZOUGHI[2], SUAD E. ABUGHRIN[3], HAGER S. EL-BESHTI[4], ESRAA A. ALHAMMALI [2], HAJER A. ALHAMMALI [2], AJAYA BHATTARAI [1,5*]**

[1] Department of Chemistry, Mahendra Morang Adarsh Multiple Campus, Tribhuvan University, Biratnagar 56613, Nepal
[2] Department of Chemistry, Faculty of Science, University of Tripoli, Tripoli P.O. Box 13503, Libya
[3]The Libyan Center for Solar Energy Research and Studies, Department of Solar cell, Tripoli P.O. Box 30454, Libya
[4] Department of Chemistry, Faculty of Science, University of Zawia, Zawia, Libya
[5] Department of Chemistry, Indian Institute of Technology Madras, Chennai 600036, India
*Corresponding author: e-mail: bkajaya@yahoo.co

**Keywords:** surface tension, surface pressure, packing parameter, ionic interactions, micelle production, cmc

The study of the interaction between aspartic acid (Asp) and cetyltrimethylammonium bromide (CTAB) reveals important information about surfactant organization, surface tension, critical micelle concentration (CMC), and surface pressure. Because of enhanced surfactant solubility brought about by electrostatic interactions, Asp's ionization lowers CTAB's CMC. The maximal surface excess concentration falls with increasing Asp concentration, suggesting competition for surface adsorption. The minimum occupied area per surfactant molecule increases at the same time, indicating changed surfactant activity at the interface between air and water. Higher CTAB concentrations are associated with a decrease in surface tension, which suggests that when Asp concentration rises, micelle production would be promoted. Saturation effects, on the other hand, happen at high Asp concentrations and interfere with micelle formation. These tendencies are supported by surface pressure measurements, highlighting the significance of ionic interactions in micelle behavior.Moreover, surfactant structuring is impacted by the packing parameter decreasing as Asp concentration increases. The changing balance between hydrophilic and hydrophobic interactions within the CTAB/Asp micellar further explained by variations in () values. The complex dynamics of ionic interactions and their impact on surfactant behavior in CTAB/Asp systems are highlighted by these studies.

# The formation of free-standing 2D crystals from amphiphilic species, the effect of counter ions

**DONG DAI, ZHIWU YU***

Department of Chemistry, Tsinghua University, Beijing 100084, China
*Corresponding author: e-mail: yuzhw@tsinghua.edu.cn

**Keywords**: DSC, SAXS, ionic liquid, two-dimensional crystal

Amphiphilic molecules can self-assemble into polymorphic aggregate structures including lamellar crystals. The preparation of two-dimensional (2D) crystals with amphiphiles, however, is very difficult.

In our laboratory, the phase behaviour of a series of amphiphilic ionic liquids composed of [$C_n$mim]X (n = 14, 16, 18; $X^-$ = $Cl^-$, $Br^-$, $NO_3^-$) was investigated recently. Various phases were indentified by employing DSC, small- and wide-angle X-ray scattering (SAXS-WAXS), and electron microscopy techniques. The phases include micellar phase, hexagonal liquid crystal phase (H), dispersed lamellar gel phase ($L_{\beta 1}$), condensed lamellar gel phase ($L_{\beta 2}$), dispersed lamellar crystal phase ($L_{c1}$), condensed lamellar crystal phase ($L_{c2}$), and dehydrated lamellar crystal phase ($L_{c3}$). Very interestingly, selection of proper anions allows the formation of widely separated 2D crystals, the $L_{c1}$ phase.

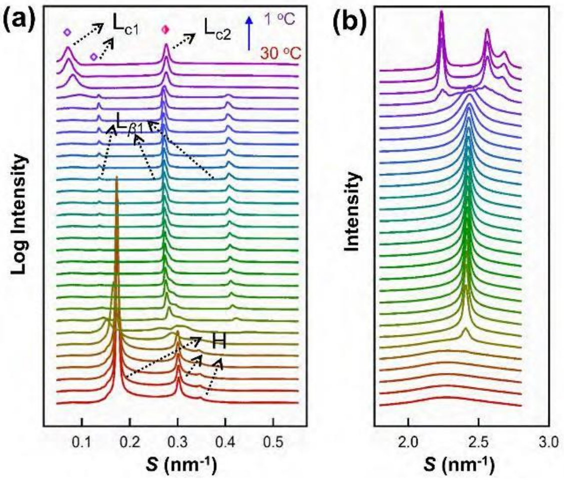


Fig. 1: Time-resolved (a) SAXS and (b) WAXS data of the 40 wt% [$C_{16}$mim]Br aqueous dispersion during cooling from 30 °C to 1 °C.

The mechanisms of the concerned phase transitions, particularly that of the crystalline phases, are discussed.

**References**
[1] D. Dai, B.B. Cao, X.L. Hao, Z.H. Li and Z.W. Yu, *J. Phys. Chem. Lett.*, 14 (**2023**) 2744.
[2] D. Dai, B.B. Cao, X.L. Hao and Z.W. Yu, *J. Phys. Chem. B*, 127 (**2023**) 7323.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Predictive structure-property correlations in semicrystalline polymers

**ALFRÉD KÁLLAY-MENYHÁRD***[1]

[1] Department of Physical Chemistry and Materials Science at Budapest University of Technology and Economics, H-1111 Budapest Műegyetem rkp. 3. H. ép. I. Hungary
*Corresponding author: e-mail: menyhard.alfred@vbk.bme.hu

**Keywords**: predictive modeling, thermal analysis, polymers, crystalline structure

The properties of the semicrystalline materials depend on their complex crystalline structure. Usually, mechanical properties especially stiffness and strength is crucial in most applications, but optical transparency and haziness are also important in the case of certain application fields. Although the key parameters of the crystalline structure, which determines the aforementioned properties, are known in the literature, the quantitative modeling is difficult and time consuming procedure if possible at all. In fact, the number of models, which link the crystalline structure to the properties, is limited in the open literature. Accordingly, prediction of upper limit of stiffness and the best achievable optical transparency is an open question in general.

In this presentation the prediction of upper modulus limit of semicrystalline polymers and the quantitative description of haze based on parameters of crystalline structure is introduced shortly. An empirical model equation was used to describe stiffness [1, 2] and the new model was developed to describe the light scattering in the semicrystalline polymers [3]. In order to model the aforementioned properties the crystalline structure was characterized in details using thermoanalytical methods, like calorimetry (DSC) and thermo-optical microscopy (TOM). A novel numerical approach was also developed to describe the crystallization process of polymeric materials in order to describe the morphology of the crystalline structure quantitatively [4]. The accuracy of the models was tested on several set of samples and good agreement was found between the calculated and measured values, however the accuracy could be improved in the future studies.

## References

[1] A. Zarbali, B. Pinke, A. Menyhárd, *Period. Polytech. Chem. Eng*. 67 **(2023)** 232
[2] A. Zarbali, I. Djaffar, A. Menyhárd, *Heliyon* 10 **(2024)**. e26122
[3] J. Molnár, Ö. Sepsi, G. Erdei, S. Lenk, F. Ujhelyi, A. Menyhárd, *J. Polym. Sci., Part B: Polym. Phys.* 58 **(2020)** 1787
[4] J. Molnár, Ö. Sepsi, B. Gaál, Z. Zuba, M. Dobrzyńska-Mizera, A. Menyhárd, *Mater. Des*. 212 **(2021)** 110245

## Acknowledgement

All the authors acknowledge financial support for Project no. TKP-6-6/PALY-2021 has been implemented with the support provided by the Ministry of Culture and Innovation of Hungary from the National Research, Development and Innovation Fund, financed under the TKP2021-NVA funding scheme.”.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Innovative Techniques for Efficient Synthesis of Amorphous Nanoscale Materials for Ultrafast Thermal Analysis

**VILKO MANDIĆ*, FLOREN RADOVANOVIĆ-PERIĆ**

University of Zagreb Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19,
10000 Zagreb, Croatia
* vmandic@fkit.unizg.hr

In recent times, the advancement of lasers with high precision and energy levels, alongside sensors boasting ultrafast response capabilities, has catalysed the emergence of ultrafast scanning calorimetry (USC). This method holds promise in unravelling and broadening our understanding of thermal and energy transitions occurring during rapid, high-energy processes like laser and plasma sintering, combustion synthesis, among others. Typically, small sample sizes offer advantages, yet they pose challenges in studying certain systems, such as soft amorphous metals, alloys, and glasses. In these cases, where micrometre-sized particles are often mixed and subjected to thermal treatment, the inherent inhomogeneity leads to poor measurement repeatability and reproducibility, rendering the results non-representative. Soft metals, though solid-state materials, exhibit a reduced level of atomic-scale ordering, whereas achieving such formations necessitates rapid cooling rates to prevent organisation. Namely, crystallization is a common occurrence during the thermodynamic cooling of molten metals. Various approaches exist to address these challenges, all falling under the umbrella of physical deposition methods given the scale of the measuring system. The crux lies in preparing minute samples homogeneously. Here, we propose a methodology for both homogeneous and precise preparation of soft metals onto USC chips, alongside a technique for the initial preparation of soft metals. Spark plasma ablation deposition (SPAD) emerges as a potent tool in this regard, igniting electrode materials into a plasma cloud that rapidly condenses into nanoparticles streamable for deposition through a nozzle. Our demonstration highlights the potential of spark ablation as a green, effective, and cost-efficient method for metallic nanoparticle production, crucial for preparing various nanocomposite materials. In SPAD, nanoparticles are generated through the disintegration of an electrode composed of the desired material, induced by a spark at high voltage in a controlled setting. This process requires only a carrier gas, an electrode, and electricity, yielding a wide range of clean metallic nanocomposites comprising multiple constituents. The cooling of particles via gas mixing induces vapour condensation, leading to the formation of atomic clusters, which subsequently coalesce into larger particles. SPAD's versatility extends to various configurations and deposition reactors, accommodating pure metals or alloys as electrodes and offering products ranging from nanoparticles to thin films, metal to metal oxide, and crystalline to amorphous structures. This investigation conclusively verifies SPAD's ability to deposit appropriate amounts and generate materials in the form of amorphous metals and to further improve USC as a measurement technique.

Acknowledgements: This work has been funded by the project UIP-2019-04-2367 by the CSF.

**T1- IL 06**

# Aggregation Behaviour of Amphiphiles in Aqueous Solutions of Various Additives

**AMALENDU PAL**

Department of Chemistry, Kurukshetra University, Kurukshetra 136119
*Corresponding author: e-mail: palchem21@gmail.com

We have investigated the micellization behaviour of cationic surfactant tetradecyltrimethylammonium bromide (TTAB) and anionic surfactant, sodium dioctylsulfosuccinate (AOT) with imidazolium based biamphiphilic surface active ionic liquid (BAIL), 3-methyl-1-pentylimidazolium dodecylsulfate [$C_5$ mim][DS] in aqueous solution, by employing various state of art techniques. The conductometry, and tensiometry measurements of TTAB with [$C_5$ mim][DS] have revealed that the micelle formation takes place at lower concentration due to strong synergistic interactions while increment in cmc value has been observed in case of AOT-[C5mim][DS] mixed system. The aggregation number ($N_{agg}$) determined for this system from fluorescence using pyrene as a probe confirms the presence of micelle/vesicles or micelles or vesicles together at different mole fraction ratio of pure components. The various surface parameters have been evaluated by using the tensiometry for both the systems. The mixed system of TTAB- [$C_5$mim] [DS] shows the enhanced surface activity in comparison to AOT-[C mim] [DS] mixed system. The size and turbidity of the mixed aggregates were investigated using dynamic light scattering (DLS) and turbiditimetry. Turbidity and DLS measurements of TTAB with [$C_5$mim][DS] have confirmed the formation of micelles as well as vesicles over an exceptionally wide range of concentration (mole fraction = 0.1- 0.9). Further, the shape and morphology of the aggregates has been studied by using the freeze scanning electron microscopy (FE-SEM) and transmission electron microscopy (TEM). The $^1$H NMR measurements shed light on the type of interactions prevail in the two oppositely charged mixed system. In case of AOT + [C5mim][DS] system, different proposed theoretical models like Clint, Rubingh and Motomura was employed for the evaluation of mixed micellar parameters(ideal values of cmc, activity coefficients of the components in the mixed micelle, and interaction parameters etc.) at different compositions. The existence of both the interactions (synergistic and antagonistic) has been inferred in this system. The mixed micelle formation was found dependent on micellar composition.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Water in Solvation Shell of Ionic Liquids: Thermodynamic, NIR Spectroscopic, Molecular Dynamics and DFT Investigations

**DILIP H. DAGADE**[1]*

[1]Department of Chemistry, Sivaji University, Kolhapur 416004, India
*Corresponding author: e-mail: dhd_chem@unishivaji.ac.in; dilipdagade@yahoo.com

**Keywords**: Ionic liquids, ion solvation, H-bonding, solvation free energy, Molecular dynamics, DFT

Energetics, structure and dynamics of ion solvation shells in aqueous medium are of crucial importance in physical and biological sciences as specificity and selectivity of ion transport (chemical or biological) is mainly controlled by the size and strength of the solvation shell which in turn depends on the strength of the H-bonds, its dynamics, kinetics and cooperative nature. Hence, in this talk, our efforts in understanding the nature of the solvation shell of ions forming the ionic liquids through experimental and computational work will be explored. Volumetric, compressibility and osmotic pressure analysis highlights the nature of ion-solvent interactions and their energetics along-with ionic hydration numbers and role of hydrophobic effect and cooperative H-bonding in explaining the higher solvation/hydration numbers than those expected theoretically based on the H-bond donors and acceptors. Molecular level understanding of these were supported and further explored using the experimental FT-NIR spectroscopic analysis where in the strength of H-bonding in the hydration shell can be associated with red or blue shift of the spectrum of water of hydration.

Experimental findings have been further detailed through DFT calculations of anharmonicity corrected NIR spectra of solvated ions and solvated hydration shell of ions along-with solvation free energy estimation both by DFT and Molecular Dynamic (MD) simulations. It has been found that the solvation free energy data excellently agrees with experimental data whenever available. The HB number, HB lifetime and the free energy of H-bond breaking where estimated using autocorrelation analysis. All these data support our experimental findings based on thermodynamics and NIR spectral data that the observed large hydration numbers are due to the cooperative H-bonding. All these investigations helps to explore our understanding of ionic solvation further and will be of high importance in the field of science and technology wherein potential use of ionic-liquids is demanded.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

---

# Thermodynamic analysis on the ionic liquid induced aggregation behavior of bile salts: An isothermal titration calorimetric approach

**HABIBA SULTANA, MAITREYEE MITRA, MAIDUL HOSSAIN, AMIYA KUMAR PANDA**

Department of Chemistry, Vidyasgar University, Midnapore-721102, West Bengal, India

*Corresponding author: AMIYA KUMAR PANDA e-mail: akpanda@mail.vidyasagar.ac.in

**Keywords**: Ionic liquid, bile salts, thermodynamics, micellization

Isothermal titration calorimetry (ITC) studies can probe concentration fluctuations as well as the thermodynamics of micellization of bile salts at different temperature. Critical micelle concentration (CMC) and enthalpy change ($\Delta H^0_{mic}$) of micellization were identified through ITC experiments directly using the phase separation model to derive the thermodynamic parameters like the Gibbs free energy change (ΔG0mic) and entropy change ($\Delta S^0_{mic}$) for two bile salts, sodium cholate (NaC) and sodium deoxycholate (NaDC). Studies were carried out under varied concentration of ionic liquid ([bmim]$BF_4$); in order to understand the effect of the counter anion, similar studies were carried out in aqueous sodium tetrafluoroborate ($NaBF_4$). Effect of temperature, in the range of 288 to 318 K, on the micellization behavior of bile salts were carried out at 1.0 mM of aqueous IL and NaBF4 solution separately. CMC values of the bile salts decreased with increasing IL and NaBF4 concentration and increased increasing temperature. CMC reduction in the NaDC-$NaBF_4$ system was more prominent, while considering temperature variation, the CMC rise in the NaC-[bmim]$BF_4$ system was more significant. Additionally, there was a considerable temperature dependency for ΔH0mic. Temperature rise caused an increase in Gibbs free energy changes, but an increase in IL and salt concentration gradually decreased the change for both NaC and NaDC. Systems showed greater spontaneity and Gibbs free energy was less affected by temperature. Entropy changes for the micellization of NaC and NaDC reveal the micellization processes to be entropy driven. Temperature had a greater effect on enthalpy change than concentration fluctuation did. As a result, in terms of temperature fluctuations NaDC in both [bmim]BF4 and NaBF4 system exhibited entropically beneficial behaviour but NaC in both IL and salts were enthalpy driven. This comprehensive study holds promise for diverse scientific and industrial applications, from pharmaceutical formulations to environmental remediation strategies.

# Solar Thermoelectric Generator with Flexible Thermal Storage

**ESWARAMOORTHY MUTHUSAMY[1]*, AMIT KUMAR BHAGAT[2]**
1,
[2] School of Mechanical Engineering, Shri Mata Vaishno Devi University, Katra 1823204, India
*Corresponding author: e-mail: m.eswaramoorthy@smvdu.ac.in

**Keywords**: thermal analysis, DSC, thermal properties

Solar thermoelectric energy-generation technology is to diminish the limitations of solar cells using better thermal management gives highly efficient and stable solar thermoelectric generators. Flexible Phase change materials (FPCMs) used to improve the performance of STEGs.

In this study, FPCM developed to investigate the heat transfer, thermal energy storage, and thermoelectric energy conversion in STEG-FPCM. Based on a parametric study, we present thermal design guidelines for the configurations of an STEG-FPCM and the thermal properties of FPCMs by considering both the thermoelectric generation performance and thermal stability of the STEG-FPCM.

The FPCM-impregnated structure is the most crucial component of the STEG-FPCM in the thermal design based on a sensitivity analysis. This study explains how FPCMs affect thermal energy transport and conversion in an STEG and sheds light on a highly efficient and stable STEG system.

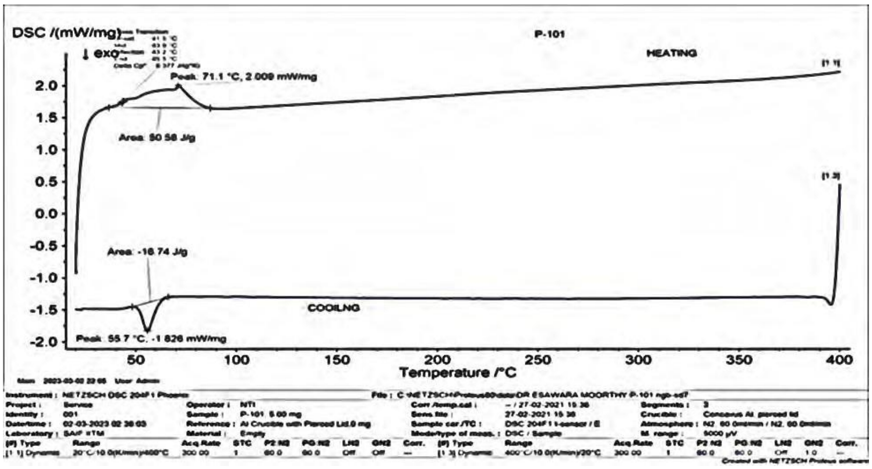


**Fig. 1 : DSC having with 15%wt of PCM and Co Polymer**

**References**

1. Dung et.al Mixed magnetism for refrigeration and energy conversion. Adv. Energy Mater 2011; 1:1215–9.
2. Presser et al electrochemical flow capacitor: a new concept for rapid energy storage and recovery. Adv. Energy Mater 2012; 2:895–902.
3. Zalba B, Review on thermal energy storage with phase change: materials, heat transfer analysis and applications. Appl. Therm. Eng., 2003; 23:251–83.
5. Sarier N, Onder E. Organic phase change materials and their textile applications: an overview. Thermochim Acta 2012; 540:7–60.*al*, 12

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Significance of measuring metabolic heats in bioprocess monitoring

**DR M SURIANARAYANAN[1]**

[1]Senior Principal Scientist and Head, CISRA-CLRI (Retired) Chennai
Corresponding author: e-mail: msuri1@outlook.com

**Keywords**: Biocalorimetry, heat flux, bioprocess monitoring, enzymes, metabolic heat.

Calorimetry excels as a process analytical tool for material and product characterization, providing insights into thermal behavior. Building upon its application in chemical reactions, biocalorimetry has been integral to bioprocess monitoring since the mid-1980s. Isothermal and heat flux calorimetry have been employed to study diverse bioprocesses, including aerobic, fermentative, and anaerobic systems. Recognizing heat as a universal metabolic byproduct, calorimetry has become indispensable for real-time bioprocess monitoring and control in recent decades. Calorimentry is foundational to quantitative bioprocess engineering and optimization. Establishing a correlation between heat generation and critical process parameters such as biomass, growth rate, enzyme activity, and substrate consumption is essential for process enhancement. This presentation delves into case studies applying metabolic heat monitoring to the production of protease, inulinase, penicillin G acylase, extracellular biopolymers, and biological dye degradation. Biocalorimetry's non-invasive, non-specific, and optically independent nature makes it a versatile analytical technique. Notably, the distinctive heat profiles (unique fingerprints heat signatures) of different organisms can be exploited to optimize bioproduct production and reduce costs.

**References**

[1] B.K. Shanmugam, S. Mahadevan, *Bioresour. Technol.* 196 (**2015**) 500–508.
[2] B. Dhandapani, S. Mahadevan, S.S. Dhilipkumar, S.Rajkumar, A.B. Mandal, *Applied Microbiology and Biotechnology* 94 (**2012**) 1533-1542.
[3] L. Santharam, A. B Samuthirapandi, S.N. Easwaran, S.Mahadevan**,** *Applied Microbiology and Biotechnology* 101 (**2017**) 1877-1887
[4] Maskow T, Paufler S. 2015. What does calorimetry and thermodynamics of living cells tell us? Methods 76:3–10.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

---

# Peptide Self-assembly -- A Hydrophobic Collapse?

**V. GANESAN, M. HAMSA PRIYA***

Bhupat & Jyoti Mehta School of Biosciences, Department of Biotechnology
Indian Institute of Technology Madras, Chennai-600036, India
*Corresponding author: e-mail: hamsa@iitm.ac.in

**Keywords**: peptide self-assembly, hydrophobic association, entropy, free energy

A net increase in the entropy of water is the classic signature of a hydrophobic association. Water molecules in the close vicinity of a hydrophobic surface possess a restricted degree of freedom, to maximize their hydrogen bonding with the environment, since there is no possibility of forming hydrogen bonds with the hydrophobic moiety. When two hydrophobic surfaces associate, the interstitial water molecules between surfaces get released to bulk solvent. Such water molecules regain more freedom, hence, the entropy of water and the system as the whole increases. Recently, in our attempt to dissect the process of self-assembly of amphiphilic peptides, we found that the interstitial water molecules between the approaching peptides in the extended conformation are also entropically restricted. Surprisingly, the molecular origin of entropic restriction results from the necessity to form a hydrogen bond bridge between two peptides. The study clearly reveals the contrasts between hydrophobic association and peptide self-assembly. Peptides tend to hydrogen bond within itself, among them and with water molecules. During self-assembly both the peptide-water and the intra-peptide hydrogen bonds get perturbed to promote inter-peptide hydrogen bonds. Our observation of high free energy cost involved in peptide self-assembly at their extended conformation provides the needed justification for the typical helix/coil to beta strand conformational transition happening during peptide self-assembly.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermodynamic properties for understanding the molecular interactions in aqueous solutions of biomolecules and drugs

**SANTOSH D. DEOSARKAR**

School of Chemical Sciences, Swami Ramanand Teerth Marathwada University, Nanded 431 606 (MS) India
*Corresponding author: e-mail: sandeo24@srtmun.ac.in

**Keywords**: volumetric properties, acoustical properties, molecular interactions

Thermodynamic properties are powerful tools to recognize the molecular interactions and hydration structure of biomolecules and drugs in solution. Drug-biomolecule interactions in solution result in significant thermodynamic changes which are reflected in thermodynamic properties. Therefore, measurement of such properties and their evaluation helps to characterize the biomolecule-drug solutions in terms of different molecular interactions and overall structural orientation. Accurately measured density and ultrasonic velocity of aqueous solutions containing biomolecule and drug at different temperatures are used for calculation of important volumetric and acoustical properties. The dependence of apparent molar properties ($V_{2,\phi}$ and $K_{S,2,\phi}$) on concentration of solute are used to determine the infinite dilution partial molar volume ($V_{2,\phi}^{o}$) and partial molar isentropic compressibility ($K_{S,2,\phi}^{0}$) of biomolecules. The transfer volumes ($\Delta_{tr} V_{2,\phi}^{o}$) and compressibilities ($\Delta_{t} K_{S,2,\phi}^{0}$) obtained from ternary to binary aqueous solutions reveals hydrophilic-hydrophilic, hydrophilic-hydrophobic and hydrophobic-hydrophobic interactions between the components in solution. The magnitude and sign of transfer properties are useful for understanding cosphere overlap of hydration spheres of solute and cosolute. In addition to this, relative viscosity and viscosity *B*-coefficients at different temperatures gives information about structure making/breaking ability of biomolecules and drugs in water. Volumetric, acoustical and viscometric properties are useful to understand the effect of added drug and temperature on hydration structure of solute biomolecule. Overall, the studies have implications in solubility, bioavailability, activity and drug delivery.

**References**

[1] V. Singh, P.K. Chhotaray and R.L. Gardas. *J. Mol. Liq.*, 220 (**2016**) 150.
[2] P. Meena and N. Kishore. *J. Mol. Liq.*, 339 (**2021**) 116718.
[3] K. Kaur, S. Arti, T.S. Banipal, and P.K. Banipal. *J. Mol. Liq.*, 330 (**2021**) 115641.
[4] S.S. Dhondge, S.P. Zodape and D.V. Parwate. *J. Chem. Thermodyn.*, 48 (**2012**) 207.
[5] S. Chauhan and K. Singh. J. Chem. Eng. Data, 59 (**2014**) 1375.
[6] N. Devunuri, S. Kancherla, B.K. Chennuri and R. L. Gardas. *J. Mol. Liq.*, 216 (**2016**) 347.
[7] S.D. Deosarkar, R.T. Sawale, R.V. Pinjari and T.M. Kalyankar. *J. Mol. Liq.*, 310 (**2020**) 113151.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Structure and Thermochemistry of Functional Metal Oxides

MARAM PARDHA SARADHI

Department of Chemistry, SRM University – AP, Andhra Pradesh, Neerukonda, Mangalagiri Mandal – 522502, India

*Corresponding author: e-mail: pardha.m@sramsp.edu.in

**Keywords**: High-temperature drop solution calorimetry, Surface Enthalpy, Configurational Entropy

My talk centred on relating microscopic features of structure and bonding to macroscopic thermodynamic behaviour in mixed metal oxides and the general problem of structure-energy-property systematics. Determining the thermophysical properties of oxides requires special calorimeters, viz., high-temperature drop solution calorimeter, Calvet-type twin microcalorimeter, ultra-high temperature DTA, drop-catch calorimeter, etc. The principles and methodologies are presented, followed by examples of applications. The thermochemical data obtained are essential to understanding materials compatibility and reactivity in technological applications, but, more fundamentally, the energetics offer insight into chemical bonding, order-disorder reactions and phase transitions. Detailed examples will be presented.

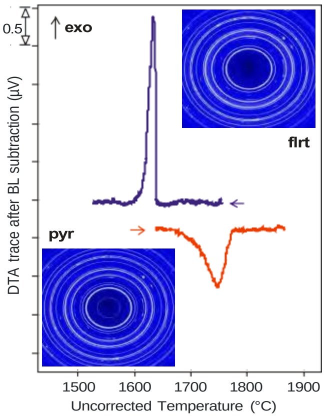


Fig: Ultra-high-temperature differential thermal analysis performed on $Sm_2Zr_2O_7$.

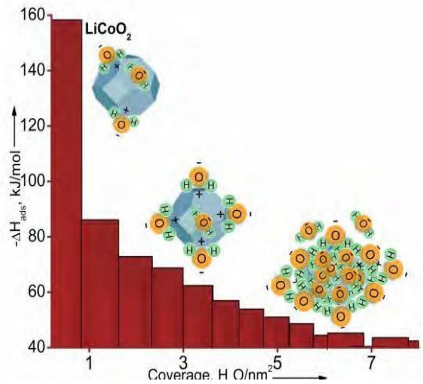


Fig. Differential $H_2O$ adsorption on nanoscale $LiCoO_2$ as a function of coverage

**References**

[1] Pardha S. Maram, Sergey V. Ushakov, Richard J.K. Weber, Chris J. Benmore, Alexandra Navrotsky, Scientific Reports, 8 (**2018**) 10658.

[2] Sergey V. Ushakov, Pardha S. Maram et. al, Adv. Appl. Ceram 117 (**2018) 582**

[3] Pardha S. Maram, Gustavo C. C. Costa and Alexandra Navrotsky, Angew. Chem. Int. Ed. 125 (**2013**) 12361

# Effect of molecular solvents on properties of imidazolium ionic liquid: Experimental and computational studies

**<u>RIYAZUDDEEN</u>*, MALIK RAIHAN AHMAD,**

Department of Chemistry, Aligarh Muslim University, Aligarh 202002, India
*Corresponding author: e-mail: rz1@rediffmail.com

**Keywords**: Ionic liquid, molecular solvent, Thermodynamic properties, Molecular Dynamic Simulation, Redlich-Kister equation; Prigogine-Flory-Patterson (PFP) theory.

The thermophysical parameters such as density, speed of sound and viscosity of pure [EMIM][MS]1-ethyl-3-methylimidazolium methylsulfate, acetonitrile (ACN), and 2,2,2-trifluoroethanol (TFE) and their binary mixture over the range of temperatures from 298.15 K to 318.15 K with difference of 5K at the atmospheric pressure 0.1 MPa has been calculated. Using these data, the parameters such as that excess molar volumes, $V^E$, isentropic compressibilities, $Ks$ deviation in isentropic compressibilites $\Delta Ks$, and viscosity deviations, $\Delta\eta$, have been determined. The derived parameters of the studied binary mixtures have been fitted to the polynomial equation, Redlich-Kister-equation. The discussion revolves around how the composition, temperature, and characteristics of the systems under study influence experimental and calculated parameters. This is examined in terms of various interactions such as ion-ion, ion-dipole, dipole-dipole and hydrogen bonding. The Prigogine-Flory-Patterson (PFP) theory has been applied to establish a correlation with the excess molar volumes of the studied binary systems.

MD simulation study examined the densities, excess molar volumes, self-diffusion coefficients, and Radial distribution function with temperatures and composition for the studied systems. In addition the coordination numbers are also derived from Molecular Dynamics (MD) simulations. This study utilizes Density Functional Theory (DFT) to investigate the interactions between pure Ionic Liquids (ILs) and their mixtures. The DFT/D3-B3LYP method is precisely employed for this analysis. This project aims to provide experimental data on the thermophysical properties and to gather information on molecular-level interactions for the systems under study. This includes ILs with same cation but varying anions and solvent molecules in binary mixtures. These interactions are understood in terms of ion-ion, ion-dipole, dipole-dipole interactions and hydrogen bonding. This holistic approach facilitates a more nuanced comprehension of the systems behaviour and properties.[1-4].

**References**

[1] Zhang, Nan-Nan Wang, *The Journal of Physical Chemistry B* 114.14 **(2010)**: 4747-4754.
[2 Lladosa, Estela, et al. *Journal of Chemical & Engineering Data* 66.2 (**2021**): 968-978.
[3] Requejo, Patricia F., et al. *The Journal of Chemical Thermodynamics* 74 (2014): 193-200.

# Phase diagram, Thermal, Structural and Optical Studies of newly synthesized Co-crystals

Sumit Chaudhary[1] and RamaNand Rai[1]*
[1]Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi-221005
*Corresponding author, E-mail: rn_rai@yahoo.co.in

Keywords: heat of fusion, phase diagram, co-crystal, solid-state synthesis, DSC

The phase diagram [1], physicochemical and thermodynamic studies of newly synthesized co-crystals [2] formed by the complexation in two organic pharmaceutical compounds namely; nicotinamide (NIC) — 3-nitrobenzoic acid (NBA) and sulfanilamide (SUL) — 3-hydroxy-4-methoxybenzaldehyde (HMB) are reported. A phase diagram is a significant study to find the precise stoichiometric ratio at which the formation of new molecular complex/co-crystal would take place. The solvent-free solid-state synthesis method [3] has been adopted for the synthesis of binary compounds in the entire range of compositions. The two novel co-crystals formed at 2:1 molar ratio in NIC—NBA and 1:1 molar ratio in SUL—HMB system along with two eutectics on either side of the co-crystal. The pure and single-phase behaviour of co-crystals and their melting are studied using DSC method. The DSC of eutectics formed in both systems are also studied. Using the experimental heat of fusion values, obtained from DSC, various thermodynamic parameters of co-crystals and eutectics have been studied and are being reported first time. Besides the phase diagram and DSC studies, FTIR, PXRD and UV–vis. absorption and emission studies also confirm the formation of co-crystals and change in their structures compared to parent components.

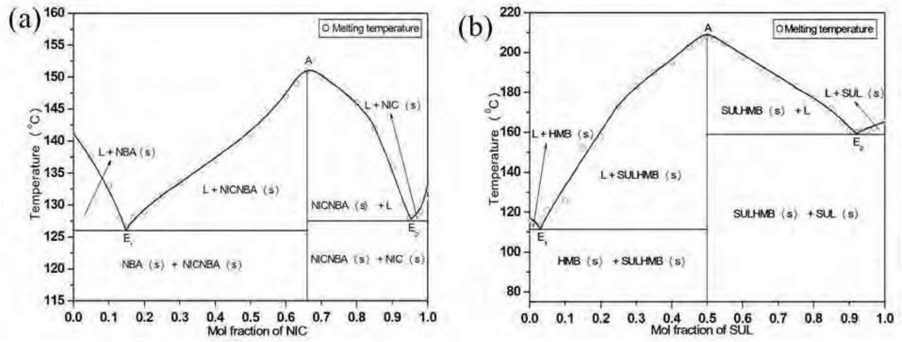


Fig. 1: Phase diagram of (a) NIC—NBA system, and (b) SUL—HMB system

References
[1] S. Chaudhary, K. Sahoo, and M. Kumar, R.N. Rai*, ACS Omega, 7(9), (2022), 7460-7471.
[2] U. Neupane, and R.N. Rai, J. Chem. Thermodyn., 161, (2021), 106513.
[3] S. Chaudhary, R. N. Rai*, D. Jyothi, U. P. Singh and A. Kumar, Mater. Chem. Phys., 322, (2024) 129541.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Recent developments to the Density marching methods for phase envelopes

**G. Venkatarathnam***

Department of Mechanical Engineering
Indian Institute of Technology (IIT) Madras, Chennai, 600036
*Corresponding author: e-mail: gvenkat@iitm.ac.in

The density marching method was introduced 10 years ago for calculating vapour-liquud isopleths [1]. The method was extended to isopleths for three phase (VLL) equilibra [2]. The method waa hen extended to P-xy diagrams. The methods have been implenented in a number of thermodynamic and process simulation software such as NIST Refprop, Aspen Plus, etc. for calculating isopleths.

We have extended this method to Global phase diagrams as well as T-xy diagrams.
In this work we present a number of complex phase envelopes including those exhibiting double azeotropy to bring out the strengths of the density marching method for phase envelopes and introduce the recent developments, which are, as yet, unpublished.

## References

1. G. Venkatarathnam, *Ind. Eng. Chem. Res.,* (**2014**) 53, 9, 3723–3730

2. G. Venkatarathnam, *Ind. Eng. Chem. Res*., (**2014**) 53, 30, 12122–12128

3. G. Venkatarathnam, *Ind. Eng. Chem. Res.,* (**2017**) 56, 46, 13894–13904

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

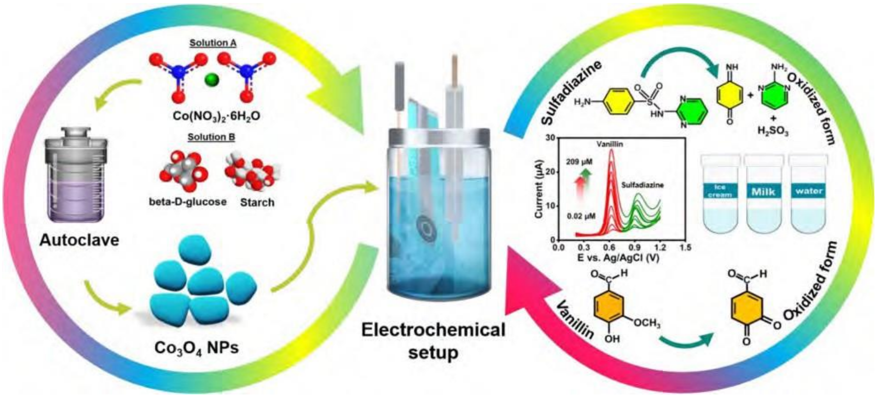
# Eco-innovative electrochemical sensing for precise detection of vanillin and sulfadiazine additives in confectioneries

**KOGULARASU SAKTHIVEL[1,2]*, GUO-PING CHANG-CHIEN[1,2], JINN-KONG SHEU[3]**

[1]Super Micro Mass Research and Technology Center, Cheng Shiu University, Kaohsiung 833301, Taiwan
[2]Center for Environmental Toxin and Emerging-Contaminant Research, Cheng Shiu University, Kaohsiung 833301, Taiwan
[3] Department of Photonics, National Cheng Kung University, Tainan, Taiwan
*Corresponding author: e-mail: kogularasu@gmail.com

**Keywords**: Vanillin, Sulfadiazine, Food additives, Green synthesis, Cobalt oxide Electrochemical sensor

The continuous emergence of food additives and contaminants in edibles, especially confectioneries, demands advanced detection methods to ensure public health and safety. Vanillin (VAL) and sulfadiazine (SD) are of paramount concern due to their extensive application in various products. While VAL is favored for its flavoring attributes, SD, a common antibiotic, can inadvertently contaminate food items. We introduced an innovative electrochemical sensor using cobalt oxide nanostructures for accurate and swift detection of these compounds. Notably, synthesizing these nanostructures through a green approach using glucose and starch is a significant advancement, offering both environmental benefits and enhanced material properties.



The novelty of the material lies in its eco-friendly synthesis route and superior electrocatalytic performance. Preliminary results indicate a promising limit of detection (LOD) VAL= 0.003 µM & SD= 0.0055 µM and a broad linear range 0.02–209 µM emphasizing its potential for real-world food quality monitoring. This work, therefore, provides a crucial intersection of sustainable material synthesis and effective food contaminant detection, heralding a new era in food safety evaluation.

## References

[1] *Applied Surface Science Advances*, Volume 20, April 2024, 100584

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# High Capacity Aqueous Redox Flow Battery

**Kothandaraman Ramanujam** *

Professor
Department of Chemistry, Indian Institute of Technology (IIT) Madras, Chennai, 600036
*Corresponding author: e-mail: rkramam@iitm.ac.in

Aqueous zinc-polyiodide (ZIFBs) flow batteries have intrinsic safety, high theoretical capacity, and energy density. But, still, ZIFBs face challenges like zinc dendrite formation, poor cyclability, water shifting, and electrolyte imbalances. This talk will exhibit how a high practical areal capacity, power density, and cycle life are achieved in our laboratory, mitigating water shifting and Zn-dendrite growth.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Graphene Based Nanocomposites for Ultra-trace Sensing

**KAMALIKA SEN*[*], DEBASHREE DAS, SHALMALI BASU**

Department of Chemistry, University of Calcutta, Kolkata-700009, India
*Corresponding author: e-mail: kamalchem.roy@gmail.com; kschem@caluniv.ac.in

**Keywords**: graphene, spectroscopy, sensing, PSA, benzaldehyde

Graphene nanoplatelets (GNPs) could be directly decorated with metal nanoparticles/composites without using any molecular linkers thereby providing new functionality to graphene. Functionalization of graphene nanoplatelet with CuI and Fe-quinoxaline nanoparticles can serve as an excellent biosensor due to their intrinsic fluorescence and Raman spectral properties. Pristine CuI nanoparticles have shown suitable band gap and photocatalytic properties. CuI functionalized GNPs (CuI-GNPs) exhibited higher efficiency towards the detection of benzaldehyde derivatives as compared to pristine CuI nanoparticles with detection limit (LOD) 2 ppm and 6 ppm for benzaldehyde and 4-methyl benzaldehyde respectively in aqueous medium. Enhanced efficacy of the prepared CuI-GNPs was also found in sensing a cancer biomarker, prostrate specific antigen (PSA) in serum medium using fluorescence spectroscopy with a 10-fold lower limit of detection (LOD) value 0.331 pg/mL as compared to CuI nanoparticles. Moreover, CuI-GNPs were found to have higher efficacy in detection of PSA in presence of 10 mM concentrations of individual interfering biomolecules like glucose and cholesterol, which are present in serum due to different comorbidities like diabetes or hypercholesterolemia. Similarly, Fe-quinoxaline nanoparticle functionalized GNPs showed Surface Enhanced Raman Spectroscopy (SERS) and offer an impressive LOD of 0.410 pg/mL.

**References**

[1] S. K. Tiwari, S. Sahoo, N. Wang, A. Huczko, *J. Sci. Adv. Mater. Dev.* **5 (2020**) 10.
[2] D. Das, N.Rana, G. Pramanik, K. Sen, *Analytica Chimica Acta* 1249 (2023) 340897.
[3] S. Basu, D. Das, Z. Ansari, N. Rana, B. Majhi, D. Patra, A. Kanungo, D. Morgan, S. Dutta, K. Sen, *Spectrochim. Acta Part A: Molecular and Biomolecular Spectroscopy* 301 (2023) 122955.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermal and Calorimetric Analyses in the Research and Development of Flame-Retardant Materials

**SUJATA MANDAL*, ANSALIN GNANA SOWNDARYA A**

Advanced Materials Laboratory, CSIR-Central Leather Research Institute, Chennai-600020, India
*Corresponding author: e-mail: sujata@clri.res.in; sujatamandal@rediffmail.com

**Keywords**: thermal analysis, DSC, metal hydroxides, cone calorimetry, leather

Flame retardancy is a critical parameter for consumer products made of textiles (natural and synthetic) and leather, specifically those used in upholstery, industrial safety wear and the strategic sector [1,2]. These materials are made fire-resistant by adding flame retardants. Flame retardants (FR) are chemicals that are incorporated into other materials during/after manufacture to retard the ignition, growth and propagation of fire, thus minimizing fire-induced destruction. They work by interfering with one or several stages of the combustion process. Therefore to develop fire-resistant materials, it is necessary to understand the combustion reaction.

Here we present the development of FR chemical(s) for leather application and the characterization of the FR chemical and the fire-resistant leather using thermal and calorimetric analyses. Most of the FR chemicals available in the market are either made with restricted substances, or produce toxic chemicals/gases on burning. Therefore, inorganic metal hydroxide-based environment-friendly and non-toxic flame-retardants are selected in the present study for making fire-resistant leathers that are used in making consumer products/goods. Various metal hydroxides and layered double hydroxides were synthesized and applied to leather. Characterization of FR chemicals and the prepared fire-resistant leathers were performed using XRD, FTIR, TGA, DSC, cone calorimeter and horizontal flammability tester.

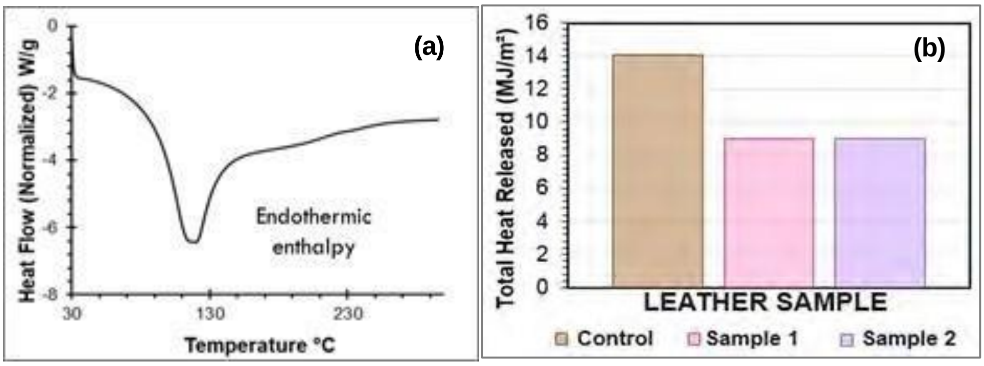


Fig. 1 (a) DSC thermogram of the FR chemical and (b) THR of the FR chemical treated leather obtained by cone calorimetry.

**References**

[1] W. An, J. Ma, Q. Xu and H. Zhang. *Composites Part A: Applied Science and Manufacturing*, 165 (**2023**) 107327.
[2] A.R. Horrocks. *Coloration Technology*, 16 (**1986**) 62.
[3] G.S.A. Ansalin, S. Mandal and R. Prasanna. *Applied Clay Science*, 230 (**2022**) 106714.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Ionic Liquids as green solvents for enhanced stability of proteins against multiple stresses

**PANNURU VENKATESU***
Department of Chemistry, University of Delhi, Delhi-110 007, India
*Corresponding author: pvenkatesu@chemistry.du.ac.in

**Keywords**: Ionic Liquids, Protein stability, Biophysical Studies, Enzyme activity, Refolding

Ionic liquids (ILs) have evolved as novel solvent systems fulfilling the requirements of biotechnology and bioengineering. In recent years, large numbers of ILs have been synthesized and their effect on protein stability has been illustrated. However, harsh process conditions, such as temperature, pH, and presence of organic solvents, are the major barriers to the effective use of enzymes in biocatalysis. We demonstrate the suitability of ILs as potential media for enzymes, in which remarkable enhanced activity and improved stability of proteins against multiple stresses were obtained. The catalytic activity of the enzyme in presence of ILs was retained against several external stimulus, such as chemical denaturants ($H_2O_2$ and GuHCl), and temperatures up to 120 °C. The observed enzyme activity is in agreement with its structural stability, as confirmed by UV–Vis, circular dichroism (CD), and Fourier transform infrared (FT-IR) spectroscopies. Finally, it is demonstrated that protein can be successfully recovered from the aqueous solution of ILs and reused without compromising its yield, structural integrity and catalytic activity, thereby overcoming the major limitations in the use of IL-protein systems in biocatalysis.

## References

[1] D. Dhimana, M. Bisht, Mara G. Freire and P. Venkatesu, *Green Chemistry,* 25 (**2023)** 650 – 660.
[2] R. Yadava, K. Kumar, S. Kumar, M. Sanjay and P. Venkatesu, *Langmuir,* 39 (**2023)** 4809–4818.
[3] U. Fatima and P. Venkatesu, *Phys. Chem. Chem. Phys.*,26 (**2024)** 14766 – 14776.
[4] C. Deepak, Indrani, A. Jayamani and P. Venkatesu, *ACS Applied Bio Materials,* 7 (**2024)** 1135–1145.
[5] D. Diksha, M. Sanjay, U. Fatima and P. Venkatesu, *Molecular Pharmaceutics,* 20 (**2023)** 3150–3159.

**T4- IL 22**

# A review on the water absorption behavior of natural fibers

**D. SAIKIA**
Digboi College, Digboi-786171, Assam, India
e-mail: dr_dip_saikia@yahoo.co.in

**Keywords**: crystallinity, diffusion coefficients, permeability, solubility.

The water absorption behavior of natural fibers was investigated under different chemical and thermal conditions by using ordinary Gravimetric absorption method. The water yielding capacity and capillarity of the fibers at constant relative humidity were measured as a function of exposure time. The various parameters of sorption process of the fibers such as diffusion coefficient, solubility coefficient and permeability coefficient were estimated. Corresponding thermodynamic sorption parameters of the fibers such as activation energy of diffusion, activation energy of permeability, change of enthalpy and change of entropy were evaluated. The effects of water absorptions on the structural characteristics of the sample under thermal conditions were also studied by using XRD, IR, TG –DTG and DSC methods. Structural and kinetic parameters were analyzed.

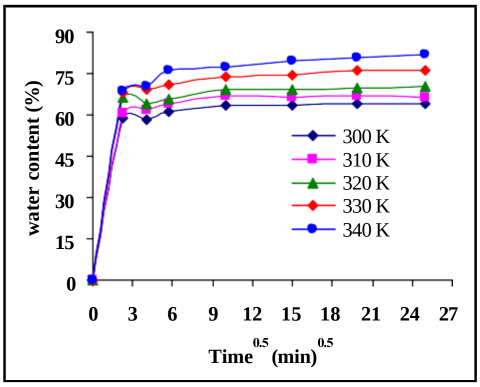


Fig. 1 : Water content absorbed by natural fibers (Abelmoschus esculentus) as a function of square root of time at different temperatures

**References**
[1] D. Saikia, *Int. J. Thermophysics*, vol. 31 (2010), pp. 1020-1026.
[2] D. Saikia, *Int. J. Thermophysics*, vol. 29 (2008), pp. 2215-2225.
[3] D. Saikia, *AIP Conf. Proc, American Institute of Physics, USA*, vol. 1004(2008), pp. 48-52.
[4] D. Saikia, M. N. Bora, *Indian Jouirnal of Pure and Applied Physics*, vol.41, (2003), pp.484-487.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Harnessing Green Nanotechnology for Industrial Solutions to Combat Antimicrobial Resistance

**ANIMA NANDA[1]* AND SHIVA SAI[2]**

[1]Department of Biomedical Engineering, Sathyabama Institution of Science and Technology, Chennai-119, India, [2] 5G Testbed, Electrical Engineering Block, Indian Institute of Technology Madras, Chennai-600036, India
*Corresponding author: e-mail: animananda72@gmail.com

## Abstract

**Keywords**: Antimicrobial Resistance (AMR), Green Nanotechnology, Antibacterial Activity, Spectroscopic Analysis, Environmental Sustainability

Antimicrobial resistance (AMR) is a critical public health threat with significant implications for health, agriculture, and economic development, particularly as India aims for Viksit Bharat by 2047. This study leverages green nanotechnology to address AMR by synthesizing silver nanoparticles (AgNPs) through an environmentally sustainable method using Bacillus subtilis, a nitrate-reducing isolate. The synthesis process was optimized by adjusting pH, temperature, concentration, and reaction time, with the resulting AgNPs characterized by spectroscopic and microscopic analyses.

The AgNPs demonstrated potent antibacterial activity against various bacterial pathogens, with FESEM and AFM analyses revealing substantial membrane damage in Gram-negative bacteria and increased surface roughness. Additionally, a 37.8% enhancement in antibacterial efficacy was observed when AgNPs were combined with antibiotics, as confirmed by UV-Vis spectrum analysis and diffraction patterns. Cytotoxicity studies on Hep G2 cells indicated apoptotic cell death, validated by DNA fragmentation and upregulated p53 expression, suggesting a mitochondrial-dependent apoptotic pathway.

Characterization of the AgNPs revealed a face-centered cubic symmetry, spherical morphology with a 22.98 nm diameter, and a surface charge of –32.3 mV. Despite these promising outcomes, challenges remain in optimizing pharmacokinetic and pharmacogenetic properties and ensuring safety through comprehensive in vivo toxicity testing. Addressing these challenges through advanced green synthesis methods and enhanced synergistic potential of AgNPs with antibiotics will pave the way for innovative industrial biotechnological solutions to AMR.

This research highlights the potential of green nanotechnology in developing sustainable and effective strategies to combat AMR, contributing to India's goal of a healthier and more sustainable future by 2047.

**References**

[1] A Nanda, M Saravanan, Nanomedicine: Nanotechnology, Biology and Medicine 5 (4), 452-456
[2] M Saravanan, A Nanda, Colloids and Surfaces B: Biointerfaces 77 (2), 214-218
[3] P Kamaraj, VV Sridhar, SV Tharumasivam, S Parthasarathy, G Bupesh, Environmental Pollution 336,
[4] MD Manoj, A Nanda, BK Nayak,Research Journal of Pharmacy and Technology 16 (7), 3183-3188

# An insight into synthetic polypeptide-based blends with other polymers: Emerging trends and advances

**MAHESH B**[1]*
[1]Department of Chemistry,
JSS Academy of Technical Education,
Dr.Vishnuvardhan Road, Bengaluru-560 060, India

*Corresponding author: e-mail: bmahesh@jssateb.ac.in

**Keywords**: Peptide-based polymer blends, Miscibility, DSC, Wound therapy

Polymeric materials are extensively used in the biomedical domain. Though it is considerably easier to use synthetic polymers in the biomedical field, natural polymers are even more required owing to their biocompatibility and biodegradability. The alternative strategy to obtain polymeric materials for biomedical applications is to blend synthetic polymers with natural ones. In this context, we wish to apprise the recent advances in peptide-based polymers and synthetic polymer blends as new biomaterials. These novel materials unveil advances in properties essential in the biomedical field. Herein, we discuss the design, preparation, structure, and physicochemical properties of the peptide-based blends with other functionally similar polymers. A few sequences of tropoelastin, such as poly(GVGVP), poly(GVGIP), poly(AVGVP), poly(AVGIP), poly[0.8(AVGVP), 0.2(AEGVP)], poly(AAGVP), reaped from the research conducted so far by our group. The physicochemical properties, such as miscibility in solid and solution phases, thermal characteristics like glass transition temperature (DSC), thermal stability (TGA), and surface morphology using SEM and AFM, are deliberated. Further focus on the potential biomedical application of these novel blends makes them suitable for wound therapeutics.

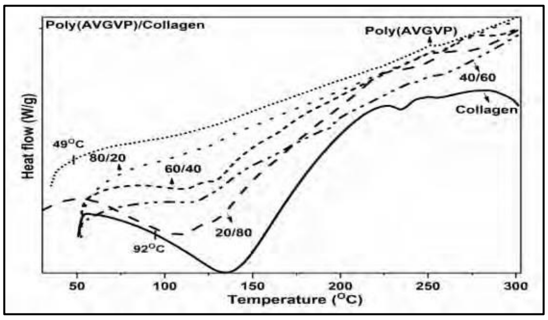


Fig. 1 : DSC showing $T_g$ of polypeptide blends with different ratios of collagen.

**References**

[1] A. Sionkowska, *Prog. Polym. Sci.* 122 (2021) 101452.
[2]. B. Mahesh, D. Kathyayani, G.S. Nanjundaswamy, D. Channe Gowda, R. Sridhar, *Carbohydrate polymers.* 129-141 (2019) 212.
[3]. A.R. Baba, D.C. Gowda, U.S. Kadimi, *Indian J. Chem. Sect. B.* 1487-1493 (2005) 44.

# Lignocellulosic Biomass to Value Added Products: Xylitol production

**SATHYANARAYANA N GUMMADI***

[1]Applied and Industrial Microbiology Laboratory, Department of Biotechnology, Bhupat and Jyoti Mehta School of Biosciences, Indian Institute of Technology Madras, Chennai 600 036, INDIA

Polyols or sugar alcohols are hydrogenated carbohydrates, which have diverse applications, particularly in food and pharmaceutical sectors. The commonly used polyols are sorbitol, mannitol, xylitol and erythritol. Xylitol is the sweetest among all the polyols, with sweetness similar to sucrose. The most attractive feature of xylitol is its non-cariogenicity. Xylitol is also shown to possess several beneficial health properties, like reducing the risk of middle ear infections in children. Several reports have emphasized the role of xylitol in enhancing bone mineralization and strength. Conventionally, xylitol is produced by chemical reduction of xylose/arabinose obtained from wood hydrolysates, which is an expensive and eco-unfriendly process. Hence, microbial production is desired.

Previously we isolated a strain from rotten apple, which is capable of producing pectic enzymes and later identified as food spoiling halotolerant yeast Debaryomyces nepalensis. This is also one among few yeast strains that utilizes both hexoses and pentoses and produces xylitol when xylose is used as carbon source. Medium optimization and microbiological parameters were optimized to enhance the xylitol production in shake flasks. Later production was studied in bioreactors and studied the effect of various process parameters on yield and productivity. Conventional optimization, artificial neural network and Genetic algorithm models also studied for enhancement of xylitol production. An attempt to convert hemicellulose hydrolysate to xylitol was studied and found that the yeast gave appreciable results. Xylose reductase is the enzyme responsible for the conversion of xylose to xylitol. The enzyme was purified and characterized and found to be halotolerant enzyme. Xylose reductase gene was also cloned and purified to homogenity. Further studies on enzymatic conversion and scale-up are under progress.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermal properties of thermochromic organic phase change materials for thermal energy storage

**KINGA PIELICHOWSKA*, NATALIA PAPROTA**

[1]AGH University of Krakow, Faculty of Materials Science and Ceramics, Department of Biomaterials and Composites, al. Mickiewicza 30, 30-059 Kraków, Poland
*Corresponding author: e-mail: kingapie@agh.edu.pl

**Keywords:** thermal analysis, DSC, phase change materials, thermochromism

Latent heat storage by phase change materials (PCMs) is one of the most preferred forms of excess energy accumulation. PCMs use the latent heat of the phase change to control temperatures within a particular range. Materials with different types of phase transition (solid-liquid, solid-solid, solid-gas, and liquid-gas) can be used for thermal energy storage. However, due to the lowest volume changes during the phase transition, PCMs with solid-liquid and solid-solid phase transitions are the most popular [1,2]. Incorporating additional thermochromic properties enables the observation of the color changes of thermochromic phase change materials (TPCMs) during the phase transition. It makes the visualization of the phase change process more intuitive and simpler [3,4].

This work aimed to investigate the thermal properties of organic thermochromic phase change materials. Thermogravimetric analysis and various types of DSC i.e. conventional, modulated and step-mode DSC were used to analyse in detail the thermal properties of TPCMs. The systems consisted of bromocresol purple as a dye, while fatty acids and fatty alcohols were used as PCMs. First, the tests included systems that, in addition to the dye, contained acid-alcohol pairs and then also three-component and four-component systems. The influence of the addition of boron nitride on the thermal and thermochromic properties of the obtained materials was also determined during the research. In the end, the obtained TPCMs have the potential to be used not only as energy storage phase change materials but also as thermoresponsive color indicators.

**Acknowledgments**

This work was supported from the subsidy of the Ministry of Education and Science for the AGH University of Science and Technology in Kraków (Project No 16.16.160.557). Research project partly supported by program „Excellence initiative – research university" for the AGH University of Krakow.

**References**

[1] K. Pielichowska and K. Pielichowski, "Phase change materials for thermal energy storage," Progress in Materials Science, vol. 65. Elsevier Ltd, pp. 67–123, 2014. Doi: 10.1016/j.pmatsci.2014.03.005.
[2] Z. Li et al., "Shape-stabilized thermochromic phase-change materials," J Thermophys Heat Trans, vol. 32, no. 1, pp. 267–270, 2018, doi: 10.2514/1.T5088.
[3] Li Z, Wu X, Wu N, Fan Y, Sun X, Song T, Zhong Q. Shape-Stabilized Thermochromic Phase Change Materials. J. Thermophys. Heat Transf. 2018. https://doi.org/10.2514/1.T5088
[4] Günther E, Hiebler S, Mehling H, Redlich R. Enthalpy of phase change materials as a function of temperature: Required accuracy and suitable measurement methods. Int J Thermophys, 2009. doi: 10.1007/s10765-009-0641-z. https://doi.org/10.1007/s10765-009-0641-z

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Our latest polymer technologies for combating climate change

**DEBASHIS CHAKRABORTY**[1]*

[1]Organometallic & Polymer Chemistry Laboratory, Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036, India
*Corresponding author: e-mail: dchakraborty@iitm.ac.in

**Keywords**: Climate change, PLA, PCHC, PBAT

Plastic pollution created by polymeric materials from petrochemical feed and climate change have a deep interconnection. The plastic characteristics are deeply altered because of rising temperatures and moisture due to climate change, resulting in the contribution of waste, generation of microplastics and release of hazardous substances into the atmosphere. It is of global importance to understand these climate driven effects and offer appropriate solutions [1]. It is completely understood that there exists a self-reinforcing cycle between climate change and pollution from plastics synthesized from monomers derived from the petrochemical feed (Fig. 1). Synthetic biodegradable polymers are the new generation of macromolecules that can mitigate the effects discussed and many of them obey the principles of "circular economy" [2].

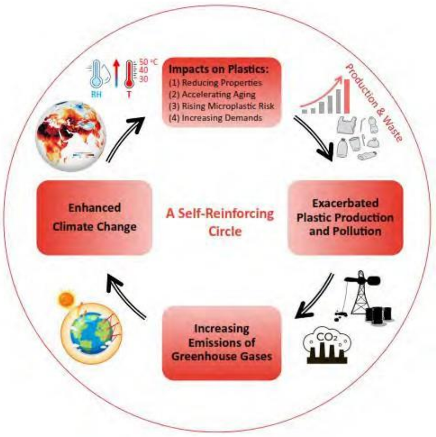


Fig. 1 : Self-reinforcing cycle between climate change and pollution from conventional plastics

Since last few years, our laboratory has conceived modern technologies (TRL-4) towards the synthesis of polylactic acid (PLA), poly(cyclohexene carbonate) (PCHC) and polybutylene adipate terephthalate (PBAT). These synthetic biodegradable polymers are in huge demand in the global market today [3].

## References

[1] X-F. Wei, W. Yang and MS. Hedenqvist, *Nat. Commun.*, 15 **(2024)** 2052.
[2] M. Lackner, B. Sajjadi, W-Y. Chen. *Handbook of climate change, mitigation and adaptation (3rd ed.)*. Springer, Switzerland AG, 2022.
[3] A. Samir, FH. Ashour, AA. Abdel Hakim and M. Bassyouni, *npj mater. degrad.*, 6 **(2022)** 68.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Characterizing the oligomerization process of the proteasomal complex from *Mycobacterium Tuberculosis*

**HEMA CHANDRA KOTAMARTHI[1]*, PUSHPKANT SAHU[1], SOHINI MONDAL[1]**
[1]Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036, India
*Corresponding author: e-mail: hemachandra@iitm.ac.in

**Keywords**: Protein oligomerization, Proteasomes, Thermal unfolding, DSC, Melting curves

Many proteins oligomerize to form functional complexes to perform enzymatic reactions. Proteases and proteasomes are complex enzymes that perform the function of protein degradation in cells and are present across various life forms. These enzymes generally have two compartments: a hexameric ATPase compartment and a tetradecameric peptidase compartment. The hexamerization of the ATPase compartment is nucleotide-driven in many proteases. However, unlike other hexameric proteases (ClpX, ClpA, etc.), Mpa, Mycobacterium Tuberculosis's ATPase, can spontaneously form hexameric complexes even without nucleotide. This is because of the stabilizing non-covalent interactions (H-bonding, electrostatic interactions, and hydrophobic interactions) among its OB domains. We have characterized oligomerization/de-oligomerization mechanisms using various bulk biophysical and biochemical studies based on tryptophan-based fluorescence emission, thermal melting, fluorescence anisotropy, native PAGE analyses, CD analyses, DSC, SEC-MALS, and DLS. We monitored the de-oligomerization and unfolding of the Mpa and proposed that the hexameric protein proceeds through a trimeric intermediate that monomerizes before unfolding.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Hybrid Two-Dimensional Porous Materials

**JAYARAMULU KOLLEBOYINA***

Hybrid Porous Materials Lab, Department of Chemistry, Indian Institute of Technology Jammu,
Jammu & Kashmir, 181221, India
Email: jayaramulu.kolleboyina@iitjammu.ac.in

**Keywords**: Coordination Polymers, Energy, Environment, Hybrids, Two-dimensional Materials

Metal-Organic frameworks are crystalline materials that comprise metallic clusters and organic ligands with great potential for a diverse range of applications, including but not limited to gas separation and storage, electrocatalysis, water purification, batteries, and supercapacitors. However, their poor conductivity, inaccessible pores, and limited stability hinder their maximum utilization. To overcome these challenges, one solution to this problem is to integrate MOFs with two-dimensional (2D) layer materials to create emerging multifunctional hybrid two-dimensional porous materials. In my presentation, I will discuss our work in integrating 2D materials to create hybrid materials with improved electro and physicochemical properties, broadening their potential applications

## References

1. K. Jayaramulu, Hybrid Two-Dimensional Porous materials, Chemistry of Materials (DOI: 10.1021/acs.chemmater.3c00829)
2. K. Jayaramulu*, S. Mukherjee, D. M. Morales, D. P. Dubal, A. K. Nanjundan, A. Schneemann, J. Masa, S. Kment, W. Schuhmann, M. Otyepka, R. Zbořil and R. A. Fischer, Graphene-Based Metal–Organic Framework Hybrids for Applications in Catalysis, Environmental, and Energy Technologies. *Chem. Rev.* 2022, 122, 24, 17241–17338

T5- IL 30

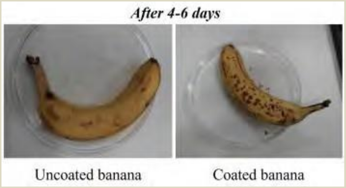
# Development of Biopolymer Based Food Packaging Films with Improved Moisture Barrier and Mechanical Properties

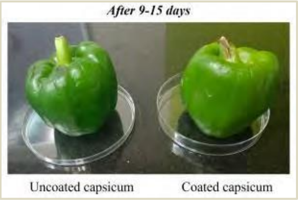
**YAMINI SUDHA SISTLA*, ABHAY KANNAN, SHUMYLA MEHRAJ**

Department of Chemical Engineering, Shiv Nadar Institution of Eminence, Delhi NCR, India.
*Corresponding author: e-mail: yamini.sistla@snu.edu.in

**Keywords**: Biopolymers, Sustainable Food Packaging, Pectin, Green Chemistry

The versatility and convenience associated with synthetic polymers have metamorphosed into a silent menace. They permeate ecosystems, leaving an indelible mark on life at every stratum. The current shift in packaging practices hinges on the strategic adoption of biopolymers derived from carbohydrates, lipids, fats, and proteins owing to their remarkable properties and ability to form uniform gels in water. Biopolymer based biodegradable films represent a significant stride in sustainable packaging solutions. The focus of the present work is to evaluate potential functional additives and optimize the process parameters to improve the moisture barrier and mechanical stability of pectin biopolymer films which otherwise in its control form tend to form moisture sensitive brittle films. Statistical design of experiments has been adopted to optimize the concentration of the functional additives. Suitability of hydrophobic and plasticizer additives such as castor oil, clove oil, bees wax, cocoa butter, *Terminalia catappa Linn*. leaf wax, cellulose nanoparticles, gluten, sorbitol, and glycerol were studied. A comprehensive comparison of properties such as water vapor permeability, water contact angle, tensile strength, elongation at break, elastic modulus, thermal degradation, melting temperature, glass transition temperature of pectin films with various combinations of additives has been carried out. *Terminalia catappa Linn*. leaf wax which has similar structure as lotus leaf significantly reduced the water vapor permeability ($2x10^{-10}$ $gm^{-1}s^{-1}Pa^{-1}$) and mechanical properties (50% elongation at break). Cellulose nanoparticles also improved the overall film performance. It was observed that higher concentrations of hydrophobic additives are critical to improve the moisture barrier properties. The conventional plasticizers which are typically hydrophilic would decrease the moisture barrier properties. Therefore, an optimum combination of the additives is essential. Furthermore, pH and concentration of the film forming solution, homogeneity of solution, temperature and relative humidity of drying, play a crucial role in over-all film properties.





References
[1] Mehraj. S, Pandey. G et al, J. Polym. Enviro. 31 (2023) 312.
[2] Mehraj S, Yamini S.S. et al., J. Polym. Enviro. 31 (2023) 3522.
[3] Mehraj. S and Yamini S. S. Elec. J. Biotech. 55 (2022) 27.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Greener Critical Mineral Extraction Methods for Sustainable Energy to Mitigate Climate Change

**SARMA V. PISUPATI*, MOHAMMAD REZAEE, YOUNES SHEKARIAN, HARI JAMMULAMADAKA, CHANDIMA SUBASINGHE, JESSE GILL**

The Pennsylvania State University, University Park, PA USA 16802
John and Willie Leone Family Department of Energy and Mineral Engineering
Center for Critical Minerals, EMS Energy Institute, 407 Academic Activities Building,
*Corresponding author: e-mail: sxp17@psu.edu

**Keywords**: critical minerals, climate change, green chemistry

The world is moving towards a net zero emission goal. The United States aims to reach net-zero greenhouse gas emissions by 2050 to limit the global temperature increase to 1.5°C. Similarly, India aims to achieve a Net zero goal by 2070. Sustainable energy options such as solar, wind, and increased EV usage for transportation are crucial to achieving this ambitious goal. Still, these options come with a steep increase in the demand for some rare earth (REEs) and critical elements. Obtaining these minerals from secondary sources, including byproducts of coal mining and other energy-based waste products and recycled batteries, is vital to developing a reliable supply chain.

Penn State has recently developed a novel process to recover these critical minerals, tested the process for proof of concept, and patented the process. The greener approach of the process has several advantages, including selective recovery of iron, aluminum, and REEs from pregnant leaching solutions using environmentally friendly chemicals and chemical-free extraction of cobalt and manganese (battery materials) to obtain high-purity products, which will render the discharge water harmless to meet the environmental regulations.

The conventional method for extracting Li from a primary mineral source of Li (i.e., spodumene) involves the conversion of naturally occurring α-spodumene to leachable $\beta$-spodumene through high-temperature calcination, followed by sulfuric acid baking, and water leaching. We have developed a patent-pending process for directly extracting Li from α-spodumene. This innovative method entails low-temperature roasting with NaOH to convert α-spodumene to soluble phases, followed by water leaching, resulting in more than 95% Li recovery. Multiple commercial Li extraction methods were tested on a Pennsylvania clay and using a shortened calcination method, followed by optimization of baking and leaching parameters, a two-stage sulfuric acid bake–water leach method was optimized for 96-99% Li extraction to a pregnant leach solution (PLS).

This presentation will discuss global research needs and ongoing efforts at Penn State in multi-metal extraction from secondary sources.

18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024

# Phytochemical Extraction of Heavy Metals (Cd & Hg) Using Orange Peel

**S. ELAMATHY, NARASINGHA NAIK, RAMESH L. GARDAS, POONGUZHALI ELAMVAZHUTHI1***

P. C. Ray Department of Chemistry, National Institute of Technology Puducherry, Karaikal – 609609,
Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036, India
Corresponding Author: e-mail: poonguzhali.e@nitpy.ac.in

**Keywords**: Extraction, Heavy Metals, orange peel, nanoparticles, pollution

The primary problem that needs immediate attention is environmental pollution which is changing climate and raising the earth temperature. The primary causes of pollution are electronic device destruction, industrial waste, and household garbage. Heavy metal waste, such as mercury and cadmium, mainly originates from industrial waste and electronic device destruction. We created an extraction method to control/prevent the heavy metal pollution in the environment, by natural product extract, synthesized ligand, and readily available chemicals which can able to make complex with heavy metals. After extracting the heavy metals from the environment can utilize for the preparation of materials as well as catalyst for the organic transformation. In order to achieve this goal, we have designed two methods [Fig. 1]. One method involves treating of the cadmium/mercury salt into orange peel extract. Another method involves the orange peel extract react with ferrous sulphate to generate iron nanoparticles, which are subsequently employed to remove the mercury and cadmium from the environmental pollution. Using both processes, the heavy metals were extracted. Using first method, reduces the chemical usage as per green chemistry principles. The extraction of heavy metals (Cd & Hg) were confirmed through SEM-EDX.

Fig. 1: Two methods for the extraction of Cd and Hg metals from environmental waste.

## References

[1] D. Mohan, H. Kumar, A. Saraswat, M. Alexandre-Franco, C. U. Pittman Jr, *J. Chem. Eng*., 236 (**2014**) 293-299.
[2] M. Fazlzadeh, K. Rahmani, A. Zarei, H. Abdoallahzadeh, F. Nasiri, R. Khosravi, *Adv. Powder Technol.*, 28 (**2017**) 122-130.
[3] K. M. Al-Qahtani, Egypt. J. Aquat. Res. 43 (**2017**) 269-274. [4] S. Bhattacharjee, F. Habib, N. Darwish, A. Shanableh, *Powder Technol*., 380 (**2021**) 219-228.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Gleanings from the synthesis of non-natural Thiamine analogues to develop novel anti-infectives.

**SUMIT BHAWAL[1]*, DIEGO A. LOPEZ[2], FRANK W. FOSS Jr[3]**

[1] Navrachana University, Vadodara-391410, India.
[2]LC R&D Scientist, Restek Corporation, Bellefonte, Pennsylvania, 16801, United States.
[3] Department of Chemistry &Biochemistry, The University of Texas at Arlington, Texas 76019, United States.
*Corresponding author: sumitb@nuv.ac.in

**Keywords**: HMP kinase, Antibacterial resistance, Thiamine, Antimetabolites

Thiamine (Vitamin $B_1$) is an essential cofactor for all organisms, but bacteria and other pathogens synthesize thiamine *de novo,* while higher organisms obtain it by dietary intake. Thus, humans lack the necessary enzymes for the complete synthesis of thiamine. Therefore, biochemical pathway exclusivity might offer target selectivity. 4-amino-5-hydroxymethyl-2-methylpyrimidine (HMP) kinase (HMP(P)K) is a unique enzyme within the thiamine diphosphate (vitamin $B_1$) biosynthetic pathway and was investigated as a potential target against bacterial infection. A series of analogues were designed and synthesized as possible substrates for HMP(P)K to understand the structure-activity relationship of HMP phosphorylation. The substrate scope was examined by an end-point luminescent kinase assay, HPLC/LC-MS, and computational docking studies. A systematic chemical modification at the C2, C4, and C5 positions of the pyrimidine ring was carried out. *C2*-substitution, furthest from the site of phosphorylation responded to phosphorylation and showed a broad range of activity. Whole cell assays indicated bacterial growth inhibition of *P. aeuroginosa, S. aureus, E. coli, K. pneumoniae* and *M. smegmatis* at micromolar concentrations for a few substrates. Metabolites of the HMP-analogues were ultimately identified from whole cells by paired ion electrospray ionization mass spectrometry PIESI-MS techniques.

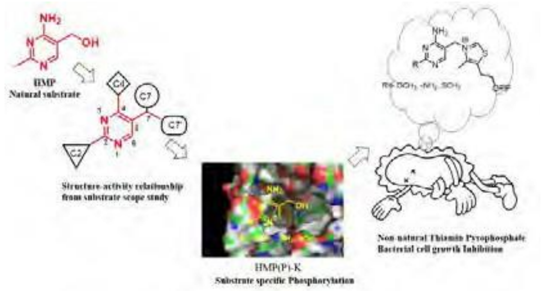


Fig. 1: Substrate scope study to investigate chemical space of HMP(P)K

**References**
[1] Jurgenson CT, Begley, TP, Ealick, SE, *Annu. Rev. Bochem,* 78 (**2009)**, 569-603.
[2] Padivitage NLT, Dissanayake MK, Armstrong, DW, *Anal. Biol. Chem,* 405 (**2013)**, 8837-8848.

T7- IL 34

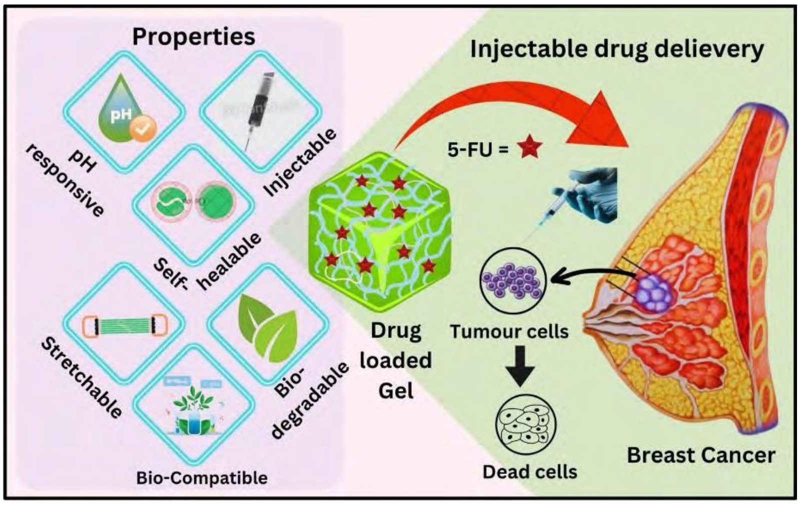
# Thermo-Responsive Multifunctional Ionic Liquid based Hydrogel as the New Age Drug Delivery Vehicles for the Treatment of Breast Cancer

**NAVED MALEK**

Department of Chemistry, Sardar Vallabhbhai National Institute of Technology, Surat- 395007, Gujarat, India
*Corresponding author: e-mail: navedmalek@chem.svnit.ac.in

**Keywords**: Drug delivery, Stimuli-responsive Hydrogel, Breast Cancer, Ionic Liquids

Developing safer, effective and targeted drug carriers with increased efficiency, low or no negative effects of drug on the healthy cells is the need of hour. Our group is developing stimuli-responsive therapeutic scaffolds that can transport drugs irrespective to their polarity to the site of action in a regulated and sustained manner. These drug carriers includes various soft assemblies including micelles, vesicles, coacervates, and hydrogels; designed from the stimuli sensitive ionic liquid (ILs). By incorporating the pH and temperature responsive surface active ionic liquid (SAIL), we have recently produced polymeric hybrid hydrogels with exceptional mechanical characteristics and unique self-healing behaviour. We have used these stimuli-responsive hybrid hydrogels as the local drug delivery system for the sustained release of antitumour drugs. We focus on the in vitro cytotoxicity and in vitro drug release study to indicate that hydrogel can be used as the targeted delivery at physiological condition and more effective in killing the cancerous cells. The newly designed hybrid hydrogel appears to be a promising candidate for local cancer therapeutics.



18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024

# Calorimetric and spectroscopic approach to evaluate solid lipid nanoparticles-based drug delivery systems

**DR. PAURNIMA TALELE**
SGGS Institute of Engineering and Technology, Vishnupuri, Nanded-431606, Maharashtra, India
*Corresponding author: e-mail: talelepaurnima@gmail.com

Keywords: Solid lipid nanoparticles, DSC, Polymorphism, crystallinity

Solid lipid nanoparticles (SLNs) are gaining considerable practical importance in pharmaceutical science for drug delivery. SLNs are attracting major attention as an alternative carrier system to traditional colloidal carriers such as –emulsions, liposomes and polymeric micro and nanoparticles. The choices of lipid, emulsifiers and their concentration have been found to affect the stability and long term storage of SLNs. The loading and release efficiency of SLNs are directly related to the local polarity within SLNs, diffusion of small molecules within the swollen lipid particles and variation of local polarities and viscosities inside the micro-heterogeneous domains of solid lipid nanoparticles. In my presentation, I will show my recent work related to development of varieties of biocompatible solid lipid nanoparticles in the form of emulsion and dry powder. Physicochemical characterization for the bulk properties like size distribution, morphology, crystallinity, polymorphism and molecular level properties like microenvironments within nanoparticles will be presented thoroughly. Thermodynamics of SLNs is studied by Differetial scanning calorimetry (DSC) and Isothermal titration calorimetry (ITC.) The drying and storage may lead to pronounced alterations in the sample properties because of temperature effects and loss of the aqueous medium. The effects may alter transition temperatures, enthalpy and polymorphism of lipids. ITC is used to study the interactions of drug loaded lipid-nanoparticles with the protein, their binding affinities with the protein. The stability and physicochemical properties of SLNs strongly depend not only on the lipid molecules but also on the nature of the stabilizers. Different compositions of lipids and stabilizers significantly affect the microenvironment by altering the micropolarity, microviscosity, and water content inside the SLNs. Fluorescent probes are highly sensitive towards their surrounding microenvironment and efficiently report the SLN properties. Different fluorescence techniques are used to characterised to SLN based drug delivery systems.

**References**

[1] D. Hou, C. Xie, K Huang, C Zhu, Biomaterials, 24 (2003) 1781–1785.
[2] W. Mehnert, K. Mader, Adv. Drug. Deliv. Rev. 47 (2001) 165–196.
[3] R. H. Muller, S. A. Runge, V. Ravelli, A. F. Thunemann, W. Mehnert, E. B. Souto, Eur. J. Pharm. Biopharm. 68 (2008) 535–544.
[4] S. A. Wissing, O Kayser, R. H. Müller, Adv Drug Deliv. Rev. 56 (2004) 1257–1272.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Assessing Microplastics Mass Concentration in the Environment by Pyrolysis–Gas Chromatography / Mass Spectrometry

**DIMITRIOS N. BIKIARIS[1]*, NINA MARIA AINALI[1,2], DIMITRA A. LAMBROPOULOU[2,3]**

[1]Laboratory of Polymer and Colors Chemistry and Technology, Department of Chemistry, Aristotle University of Thessaloniki, GR-541 24, Thessaloniki, Greece
[2]Laboratory of Environmental Pollution Control, Department of Chemistry, Aristotle University of Thessaloniki, GR-541 24 Thessaloniki, Greece
[3]Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Balkan Center, Thessaloniki GR-57001, Greece
*Corresponding author: e-mail: dbic@chem.auth.gr

**Keywords**: microplastics, Py–GC/MS, mass concentration, wastewater treatment plant.

Microplastics (MPs) have been detected across various ecosystems globally, highlighting the necessity for a comprehensive assessment of their distribution patterns and the establishment of risk evaluation protocols. In recent years, wastewater treatment plants (WWTPs) have emerged as active transport pathways for MPs due to the limited efficacy of conventional treatment facilities in removing plastics, thus significantly contributing to the dispersion of MPs into aquatic environments. Understanding and mitigating the presence of MPs in WWTP effluents are crucial for preserving ecosystem integrity. Yet, the understanding gained regarding the quantity, removal, and influence of MPs in WWTPs primarily relied on particle count rather than mass. Particle count, in contrast to mass, inadequately characterizes the extent of MP pollution due to their size variability spanning three orders of magnitude. Furthermore, MPs may undergo fragmentation during physicochemical processes, potentially influencing particle count and leading to an overestimation of their concentration. Within this context, the present study focused on examining the occurrence and composition of MPs in effluents from a Greek WWTP located in Thessaloniki over a one-year period, aiming to elucidate their temporal impact on receiving water bodies. Microscopy aided in categorizing suspected MPs, while pyrolysis gas chromatography/mass spectrometry (Py–GC/MS) analysis facilitated identification and mass concentration determination of MPs. Fibers predominated as the primary form of MPs (50-78%) compared to particles. Py–GC/MS analysis identified polyolefins as the dominant polymer type, along with quantifying MP concentrations, showing increased MP levels after rainfall events and windy conditions, emphasizing the importance of considering background parameters in future MP monitoring strategies.

**Acknowledgments**
This work has been financially supported by the Greek Ministry of Development and Investments (General Secretariat for Research and Technology) through the research project “Intergovernmental International Scientific and Technological Innovation-Cooperation. Joint declaration of Science and Technology Cooperation between China and Greece” (Grant no: T7ΔKI-00220) and it is gratefully acknowledged.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Application of thermal analysis in the development of biomass valorization technologies

**DEEPAK KUMAR OJHA***

Department of Chemical Engineering, Indian Institute of Technology Roorkee, Roorkee-247667, India
*Corresponding author: dojha@ch.iitr.ac.in

**Keywords**: Thermal analysis, analytical pyrolysis, biomass-coal combustion

This abstract presents two significant studies delving into biomass transformation processes, emphasizing the pivotal role of thermal analysis in understanding these phenomena.

Firstly, a comprehensive examination of lignocellulosic biomass combustion is conducted, employing thermal analysis techniques to explore ignition properties, energy dynamics, and mass transport limitations across pyrolysis, gasification, and oxidation stages. Through meticulous thermogravimetric analysis and isoconversional methods, the study unravels the influence of pyrolysis on overall combustion dynamics. Differential calorimetry unveils distinct exothermic zones dominated by volatile combustion, shedding light on fundamental aspects of biomass combustion. Furthermore, Fourier-transform infrared spectroscopy (FTIR) elucidates structural transformations, offering deeper insights into biomass behavior under thermal stress.

In parallel, another study investigates the impact of gamma radiation exposure as a pretreatment technique on rice straw valorization. Employing advanced analytical pyrolysis technology coupled with thermal analysis, the study uncovers significant alterations in functional group composition and crystallinity induced by radiation exposure. Notably, thermal analysis during fast pyrolysis reveals enhanced carboxylic acid production post-exposure, indicating radiation-induced modifications in chemical reactivity within rice straw. These findings underscore the critical importance of thermal analysis in elucidating the transformative effects of gamma radiation on biomass composition and valorization potential. These studies underscore the interdisciplinary nature of biomass research and highlight the pivotal role of thermal analysis in advancing our understanding of biomass pretreatment and valorization strategies.

### References

1. Meena, M.K; Anand, S.; Ojha, D.K., *Journal of Analytical and Applied Pyrolysis, J. Therm. Anal. Calorim.* 148 (**2023)** 5509.
2. Meena, M.K.; Bhaskar, T.; Gourishetty, A.K., Ojha, D.K.;,*Int. J. Green Energy*, **2023**

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Uncovering the potential of aqueous solutions of deep eutectic solvents on the extraction and purification of collagen type I from Atlantic codfish (Gadus morhua)

**MEENA BISHT, [1] * MARGARIDA MARTIN[2], C. R. V. DIAS[2], SÓNIA P. M. VENTURA[2]* AND JOÃO A. P. COUTINHO[2]**

[1]Department of Chemistry, Sri Venkateswara College, Dhaula Kuan, New Delhi, Delhi 110021
[2]CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro,
3810-193 Aveiro, Portugal.
*Corresponding author: e-mail: meena@svc.ac.in, spventura@ua.pt

**Keywords**: circular economy, green solvent, deep eutectic solvent, collagen

Marine fish industries discard huge amounts of fish waste every year, which in turn impose problems of environmental pollution and loss of economic value.[1,2] About 75% of the total weight of fish is discarded in the form of skins, bones, fins, heads, guts, and scales, which contain high levels of collagen type I. Generally, major sources for commercial collagens are the skin and bone of pigs and cows; however, these sources are chiefly associated with the risk of transference of zoonotic diseases or religious issues.[3,4] Traditional protocols applied to the extraction of collagen are outdated, mainly with respect to present demands to develop more sustainable processes. This work explores the use of sustainable solvents, such as deep eutectic solvents (DES), to develop a more efficient, cost-effective and biocompatible process to extract collagen from waste from the fish industry waste. The extraction of collagen from the skin of Atlantic cod (Gadus morhua) using aqueous solutions of various eutectic solvents was studied, and after selection of the best solvent, an aqueous solution of urea (U) and lactic acid (LA) at a molar ratio of 1 : 2 (U : LA 1 : 2), the collagen extracted was properly characterized using SDS-PAGE, CD, FTIR, and XRD, and shown to be of type I. The results obtained here demonstrate an improvement in the yield and quality of the extracted collagen when eutectic mixtures were applied instead of acetic acid. After optimization of the process conditions, a maximum extraction yield of 6% was obtained for the aqueous solution of U : LA 1 : 2 at 0.75 M. The present work demonstrates the potential use of codfish skin waste and an aqueous solution of a DES to develop a more environmentallyfriendly process to obtain high-quality collagen type I. It is an effort to convince industries to valorize their own residues under the guidelines of a circular economy.

**References**

[1] F. M. Kerton, Y. Liu, K. W. Omari and K. Hawboldt, Green Chem., 15 (2013) 860.
[2] X. Cheng, Z. Shao, C. Li, L. Yu, M. A. Raja and C. Liu, PLoS One, 12 (2017) e0169731.
[3] D. J. Prockop and K. I. Kivirikko, Annu. Rev. Biochem., 64 (1995) 403–434. [4] J. A. Hodges and R. T. Raines, J. Am. Chem. Soc., 125 (2003) 9262–9263.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Powering Tomorrow: Innovative Gas Hydrate Technologies for a Sustainable Future

GAURAV PANDEY

Department of Petroleum Engineering and Earth Sciences, Energy Cluster, School of Advanced Engineering, UPES, Dehradun, Uttarakhand-248007, India

*Corresponding author: gaurav.pandey@ddn.upes.ac.in

**Keywords**: gas Hydrates, sequestration, clean energy, rheological, kinetics

The surge in global greenhouse gas emissions (mainly $CO_2$) has introduced the world to the significant problem of climate change. A paradigm shift towards sustainable energy sources is necessary to meet the sustainable development goals (SDGs). Natural gas hydrates are ice-like crystalline solid compounds formed by (host) water molecules, in which the guest (gas) molecules are trapped inside the water cavities. Generally, these guest molecules are methane, ethane, propane, and carbon dioxide, etc. Natural gas hydrates have achieved considerable significance due to their potential role as a future clean energy resource. To improve the kinetics and gas consumption of hydrates system, various kinetic promoters are used such as sodium dodecyl sulfate (SDS), tetrahydrofuran (THF), etc. A novel approach to hydrate-based $CO_2$ capture and sequestration has gathered significant attention due to its potential to provide long-term $CO_2$ sequestration and hydrogen storage using hydrogen hydrate technology. Herein, the methane-carbon dioxide sweeping process ($CH_4$-$CO_2$ replacement) has gained considerable interest as it produces clean energy (natural gas) from natural gas hydrate deposits while sequestering anthropogenic $CO_2$. Implementation of CCS involves enormous capital expenditure along with transportation, sequestration, and purification costs making its adaptability economically unfeasible. In this regard, the morphological, kinetics and rheological studies of hydrate systems have gained interest to carried out research for storage and flow assurance applications for a sustainable future.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Making $CO_2$ Capture and Sequestration one of the Most Sustainable Path for Net Zero World

**Rajnish Kumar***

Department Chemical Engineering at IIT Madras
*Corresponding author: e-mail: rajnish.ncl@gmail.com

Global $CO_2$ emission has touched 37.5 billion tons of carbon dioxide per year, and despite all the talk about net zero $CO_2$ emission, the rate of $CO_2$ emission is expected to stay at the current level for few more years. While role of solar, wind, hydro/waves, hydrogen etc. (perhaps nuclear as well) is acknowledged, current energy need, and proposed GDP growth of developing countries could not be achieved without ensuring implementation of CCUS. CCUS is essentially a three-step process, i) Capturing or separating the $CO_2$ from its associated gases, ii) Transporting the captured, relatively purer $CO_2$ (from step-i) to the utilization site where part of the $CO_2$ could be processed for its utilization, and iii) Majority of the $CO_2$ which could not be converted (in step-ii) has to be transported and sequestered for geological timescale. Thus, amount of $CO_2$ utilized or sequestrated is directly proportional to the amount of $CO_2$ captured. $CO_2$ capture technology has to become robust, and sustainable with time, this presentation would briefly explain gas hydrates at molecular level, and its potential application in achieving net zero carbon dioxide emission. Focus would be on explaining a) What is a gas hydrates-based $CO_2$ capture and sequestration process? and b) Why this process is one of the most sustainable process compared to other mature technologies currently being used for $CO_2$ capture?

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Creating and Including Open Educational Resources in the Era of Digital Education and Outreach

**ARUN K. TANGIRALA ***

Professor
Department of Data Science and Artificial Intelligence,
Indian Institute of Technology (IIT) Madras, Chennai, 600 036
*Corresponding author: e-mail: arunkt@iitm.ac.in

Formal education and learning, traditionally, for centuries have been geographically confined to schools or university campuses. This model has withstood the test of time and has been adopted globally with great success. However, it has also resulted in regionalising and increasingly restricted access to quality education to the affordable. Further, it has quite often led to unhealthy competitions in several scenarios. With the excellent advances in digital communication, educational technologies and the advent of artificial intelligence, we stand at a juncture to witness a paradigm and monumental shift in the mode of education. This unprecedented shift has an enormous potential in breaking the barriers of geography and financial affordability, thereby bridging the gap between earnest learners and the abodes of education. While digital technology provides the communication platform, educational technologies bring tools to handle the diversity of learners, and AI equips us with the tools to handle large-scale assessment / personalised learning. SWAYAM PRABHA (SP), an educational outreach initiative of the Ministry of Education, GoI, is a large-scale educational content creation and dissemination project. A multi-institutional project, SP actively creates multi-lingual content for higher education in all disciplines including arts, humanities, sciences, engineering and skills using the DTH and Internet platforms for dissemination. This talk presents an overview of this large-scale project and underlying efforts with focus on sciences including chemistry. In addition, the talk will briefly discuss the road ahead on adopting such open educational resources in university / classroom education.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Learning How to Teach

**EDAMANA PRASAD***

Professor
Department of Chemistry & Head, Teaching Learning Centre (TLC),
Indian Institute of Technology (IIT) Madras, Chennai, 600 036
*Corresponding author: e-mail: pre@iitm.ac.in

The Indian Institute of Technology (IIT) Madras, established in 1959, has developed into a premier institution for science and engineering education, earning recognition both nationally and internationally for its excellence in teaching and research. Teaching-Learning Centre (TLC) at IIT Madras has been functioning as an independent centre since 2011. The centre is dedicated to enhance the quality of teaching and learning by fostering continuous improvement and innovation in instructional methods. Its primary objectives are to elevate teaching practices through professional development, support effective learning environments that cater to diverse student needs, and integrate cutting-edge educational technologies. The TLC achieves these goals by providing faculty with access to the latest pedagogical research, organizing training workshops on new teaching tools and methodologies, and encouraging collaboration to share and implement successful practices. Additionally, the centre focuses on evaluating and refining educational strategies to improve student performance and engagement, thereby promoting a culture of excellence and ongoing enhancement in higher education.

The talk will briefly summarize the activities of the centre, emphasizing on the need for a paradigm shift in teaching learning process in higher education, and expected to leave the audience with ‘food for thought’ on future education approaches.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Application of thermodynamics for discovery of potential inhibitors for disease associated protein targets

**SINJAN CHOUDHARY***

UM-DAE Centre for Excellence in Basic Sciences Mumbai
*Corresponding Author e-mail: sinjan.choudhary@cbs.ac.in

A key part of drug design and development is the optimization of molecular interactions between a drug/inhibitor and its binding target. For the drug discovery scientist, the term “thermodynamics” refers to the study of the heat change that occurs when biomolecules interact. It can be measured either directly by isothermal titration calorimetry (ITC) or indirectly by using any technique that can be used to determine an affinity over a range of temperatures such as fluorescence spectroscopy. Thermodynamic characterization provides information about the balance of energetic forces driving binding interactions and is essential for understanding and optimizing molecular interactions. The most effective drug design and development platform comes from an integrated process utilizing all available information from structural, thermodynamic and biological studies. We have made an attempt to integrate thermodynamics with spectroscopy and molecular docking to find potent inhibitors against the disease associated proteins α-Synuclein and plasmepsins. Structurally, α-Synuclein is an intrinsically disordered protein present in the nerve cells whose aggregation is linked with Parkinson’s Disease. On the other hand, plasmepsins belong to aspartate proteases and are present in the malarial parasite Plasmodium. The inhibition of the activity of plasmepsins leads to parasitic death and hence can be used as a drug target for antimalarial therapy. The energetics of interactions obtained from ITC provides information about the nature of interactions involved the binding of inhibitor with the target protein. This information is integrated with the molecular docking studies to know about the amino acids and functional groups involved in the binding and inhibition. These findings can help in the establishment of structure-energetics-function-inhibitory activity relationship and will provide guidelines for the design/modification of inhibitors in future drug development.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Ionic Liquids and Deep Eutectic Solvents: Applications in Materials Chemistry and Biomass Processing

**ARVIND KUMAR***

Chief Scientist & Divisional Chair, Salt and Marine Chemicals Division
CSIR-Central Salt and Marine Chemicals Research Institute G. B. Marg, Bhavnagar-364002, Gujarat (India)
Email: arvind@csmcri.res.in

**Keywords**: Ionic Liquids, Deep Eutectic Solvents, Colloidal Chemistry, Nanomaterials, Biomass

Ionic liquids (ILs) are the organic analogues of inorganic molten salts with melting temperature < 100°C, whereas deep eutectic solvents (DESs) are formed from a eutectic mixture of Lewis or Brønsted acids and bases which can contain a variety of anionic and/or cationic species, and now widely acknowledged as a new class of ionic liquid (IL) analogues. ILs and DESs have wonderful solvent properties such as low volatility, high thermal stability, wide liquid range and good solvating ability. Superior physicochemical properties distinguish ILs and DESs from conventional organic solvents, and are fast replacing these in different chemical applications.

Present work is focused on two distinguished applications of ILs and DESs viz. colloidal formulations for advanced materials and biomass processing for separation/depolymerization of biopolymers. We have shown that by using ILs/DESs as a medium and surfactant highly thermally stable self-assembled structures can be constructed. These structures have been used as ionic nanoreactors for preparation of shape/size controlled nanomaterials/quantum dots, metal organic frame works (MOFs) suitable for advanced applications.[1,2] In an another application, the use of ILs/DESs in biomass processing for clean separation of biopolymers (cellulose, hemicellulose and lignin) and recovery of other value added chemicals has been shown. We have developed strategies to depolymerize the biopolymers at ambient conditions, for example lignin has been valorized efficiently using metal based ionic liquid systems in order to convert value added chemicals.[3,4] Biopolymers dissolved in ILs/DESs have been utilized to prepare ion gels/composite films for biomedical and soft matter devices.[5]

**References**

[1] P Bharmoria and A Kumar* *Chem. Commun.,*, 52, 2016, 497-500.
[2] K Damarla, Y Rachuri, E Suresh, and A Kumar,* *Langmuir*, 2018, 34, 10081−10091.
[3] Mohit J. Mehta, Akshay Kulshrestha, Shweta Sharma and Arvind Kumar, * *Green Chemistry*, 2021, 23, 1240–1247.
[4] K Singh, M K Paidi, AKulshrestha, P Bharmoria, S K Mandal, A Kumar,* Separation and purification techonlogy, 2022, https://doi.org/10.1016/j.seppur.2022.121636.
[5] T J Trivedi, D Bhattacharjya, J-S Yu, A Kumar,* *ChemSusChem.* 2015, 8 (19), 3294 – 3303.

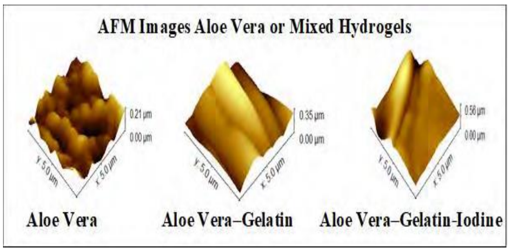
# Towards Development of Aloe Vera Based Hydrogel Iodophors as Antiseptic Agents: A Reappraisal

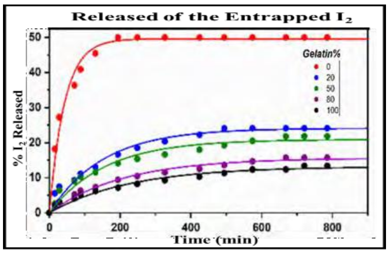
**Homendra Naorem**

Department of chemistry
Manipur University, Canchipur, Imphal-795003, Manipur, India
e-mail: naorem.homendra@gmail.com

**Keywords**: Iodophor, Aloe Vera, Gelatin, HPC, Entrapment, Sustained Release

Iodophors are preparations containing iodine complexed with a polymer that serve as sustained release reservoir of iodine which can effectively be used as broad spectrum biocidal agents. In view of the healing properties and the bio-compatibility, we have investigated if Aloe Vera gels can be a good iodophor. Aloe Vera gel weakly interacts with iodine which limit its complexation and hence entrapment ability of iodine. Aloe Vera gel can entrap about 12% of available iodine which is released fast in about 3 h when immersed in pure water implying that Aloe Vera alone will not act as good iodophor. On the other hand, gelation (15%) or HPC (6%) hydrogels can entrap about 64 or 20% iodine, out of which about 13 or 36% of the iodine entrapped in gelatin or HPC hydrogel can be steadily released over a period of 13 or 30 h respectively. The iodine entrapment ability of Aloe Vera can be significantly improved from about 13 to 30% by blending it with gelatin or HPC hydrogels. The blended hydrogels showed slow and sustained release of the entrapped iodine – increasing from 3 h for pure Aloe Vera to more than 10 h for the blended hydrogels.


AFM Images Aloe Vera or Mixed Hydrogels


Released of the Entrapped $I_2$

The pure or the blended hydrogels were characterized using FTIR, SEM, EDAX, XRD, AFM, etc. techniques. The AFM images showed no significant changes in the topographies of the pure or the blended hydrogels with or without iodine except an increase in the surface roughness in the blended hydrogels which decreased with the entrapment of iodine implying that iodine may be involved in the crosslinking in the hydrogels. It was observed that the entrapment of iodine initially followed Freundlich isotherm. Preliminary studies showed that iodine entrapped in the blended hydrogels exhibited better the antibacterial properties as compared to the unblended hydrogels.

**References**

[1] D.N. Makhayeva, GS Irmukhametova, VV Khutoryansky, Rev J Chem 10 (2020) 40.
[2] H. Naorem, N. Subhaschandra Singh, J. Phys. Chem B 111, (2007) 4098
[3] H. Naorem and S D Devi, Spectrochim Acta Part A: Mol and Biomol Spec 101, (2013) 67

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Solvation Behavior of Some Bioactive Compounds in Aqueous and Aqueous Solutions of Dextrose and Urea Solutions

**SUDHAKAR S. DHONDGE[1]*, RAVIN M JUGADE[2]**

[1]1Department of Chemistry, Seth Kesarimal Porwal College, Kamptee, Nagpur- 441001, India
[2]Department of Chemistry, Rashtrasant Tukadoji Maharaj Nagpur University, Nagpur - 440033
*Corresponding author: e-mail: s_dhondge@hotmail.com

**Keywords**: Volumetric Properties, Compressibility properties, Bioactive Compounds

Human body is extremely complicated machine. Several physical, chemical and biological reactions are taking place in it simultaneously and precisely. So, it is difficult to understand the behaviour of all these compounds in aqueous solutions simultaneously. However, they can be studied individually. Thermodynamic properties are generally convenient parameters for interpreting solute-solvent and solute-solute interactions in the solution phase. In this study, volumetric and compressibility behaviour of Creatinine, Ornithine hydrochloride and Citrulline in aqueous and aqueous solutions of Dextrose and Urea at different temperatures has been discussed. In aqueous binary solutions, dextrose acts as a structure maker, whereas, urea acts as a structure breaker. But, all the solutes act as structure breakers in aqueous as well aqueous solutions of urea and dextrose at all the studied temperatures. It has been observed that apparent molar isentropic compression is negative for all the systems, at all the temperatures. It suggests that when these solutes are dissolved in water, the aqueous layer around solute becomes less compressible.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Deep Eutectic Solvents as Novel Thermal and Separation Media: Insights from Quantum Chemical and Molecular Dynamics Simulations

**TAMAL BANERJEE**

Department of Chemical Engineering, IIT Guwahati, Guwahati 781039, India
*Corresponding author: e-mail: tamalb@iitg.ac.in

**Keywords**: Deep Eutectic Solvents, Aromatic Extraction, Nanofluid, Thermal conductivity

The talk shall discuss Molecular Dynamics (MD) and Quantum Chemistry (QC) computations for aromatic extraction by Deep Eutectic Solvents from aqueous and hydrocarbon streams respectively. Distinct Deep Eutectic Solvents (DESs) consisting of hydrogen bond acceptor (HBA) and hydrogen bond donors (HBDs) have been adopted as solvents[1]. Using MD simulations, the non-bonded interaction energies along with the radial, combined, and spatial distribution functions were determined, highlighting the improved and beneficial interactions of DES components with aromatic moieties. Bader's Quantum Theory of Atoms in Molecules (QTAIM) was then adopted to reveal the nature of such interactions. The simulation was used to calculate distribution coefficient, selectivity and extraction efficiency. This was then compared with experimental liquid liquid equilibrium measurements. Futher a variant, namely Natural Deep Eutectic Solvents (NADESs) have also emerged as promising materials for the formulation of nanofluids[2] comprising of Betaine (Be) as HBA with Lactic acid (LA) and Ethylene glycol (EG) as HBD. The thermal conductivity of both the nanofluids was almost 7-9% higher (0.21-0.25 W/mK) than that of the base fluid, and with an increase in the volume fraction (0.01-0.05) of the nanoparticle. Further the predicted thermal quantities were also compared with those from MD simulations.

## References

[1] Naik, P, K; Kumar, N, Paul N, Banerjee, T. (2022).ISBN: 9781003231158.CRC Press.

[2] P. Dehury, U.Mahanta, R. Singh, and T.Banerjee, *Journal of Molecular Liquids*, *379* (**2023**) 121700.

# Effect of Additives on the Solution Behavior of Surfactants

**MD. SAYEM ALAM** [1]*

[1]Polymer Science and Technology Unit, Advanced Materials Laboratory, Council of Scientific and Industrial Research (CSIR) — Central Leather Research Institute (CLRI), Adyar, Chennai 600 020, India.
*Corresponding author: e-mail: sayemalam@gmail.com, sayem@clri.res.in.

**Keywords**: surfactants, critical micelle concentration, clouding phenomena, thermodynamics, leather chemicals

The surfactants (Fig. 1) are amphiphilic molecules that contain two parts: non-polar (oil preferring or water fearing part, referred to as lipophilic or hydrophobic), and the other one is polar (water preferring part, hydrophilic) part. In aqueous environment, surfactant molecules can form a kind of self-organized molecular assembly above their critical micelle concentrations (CMC) which can be called as micelles (Fig. 1) [1-3]. The self-assembly and self-organization (or micellization) is a natural and spontaneous processes. The micellization processes is occurring mainly through non-covalent interactions (such as, van der Waals, hydrogen bonding, hydrophobic/hydrophilic, electrostatic, donor and acceptor, and metal-ligand coordination networks). The interests in micelle solutions stems from their potential as functional molecular assemblies for use in many fields of pure and applied sciences as they can be used as models for several biochemical and pharmacological systems. The self–association / mixed micellization, the clouding or cloud point (CP) [4,5], and the thermodynamics of amphiphilic molecules in the absence and presence of additives were investigated.

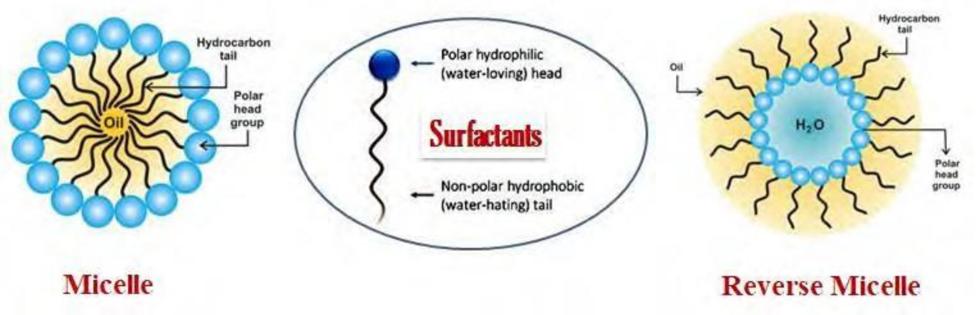


Fig. 1 : Cartoon presentation of surfactant, micelle and reverse micelle.

**References**

[1] Rosen, M. J.; Kunjappu, J. T., *Surfactants and interfacial phenomena*. John Wiley & Sons: 2012
[2] Alam, M. S.; Mandal, A. B. *Journal of Molecular Liquids* **2012,** 168, 75-79.
[3] Alam, M. S.; Siddiq, A. M.; Natarajan, D.; Kiran, M. S.; Baskar, G. *Journal of Molecular Liquids* **2019,** 273, 16-26..
[4] Alam, M. S.; Mandal, A. B. *Journal of Chemical & Engineering Data* **2010,** 55, (5), 1893-1896.
[5] Alam, M. S.; Mandal, A. B. *Journal of Molecular Liquids* **2015,** 212, 237-244.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Unveiling the Molecular Interactions of Ionic liquids and Drugs in aqueous Solutions through Volumetric and Compressibility Insights

**SANGESH P. ZODAPE***

Department of Chemistry, Visvesvaraya National Institute of Technology (VNIT), Nagpur- 440 010, Maharashtra, India
*Corresponding author: e-mail: szodape@chm.vnit.ac.in, sangesh02@gmail.com

**Keywords:** Density; Speed of sound; Limiting apparent molar volume; Limiting apparent molar isentropic compressibility.

Molecular interactions are important in chemistry, biology, and materials science because they influence the behavior and properties of complex systems. Understanding these interactions at the molecular level is critical for pharmaceutical design and optimization, the development of new materials, and the understanding of biological processes. This research delves at the nature and impact of molecular interactions, including hydrogen bonding, van der Waals forces, electrostatic interactions, and hydrophobic effects. The interactions between drug molecules and ionic liquids, which are increasingly being used as versatile solvents in pharmaceutical formulations, are highlighted in particular.

Understanding the volumetric and compressibility properties of pharmaceuticals, ionic liquids and drug-ionic liquid in water is critical to the advancement of pharmaceutical science and the creation of novel drug delivery systems. These characteristics significantly influence drug solubility, stability, and bioavailability. Volumetric qualities, such as molar volume, limiting apparent molar volume and expansivity, provide information about molecular interactions and structural traits, which are necessary for developing effective pharmacological formulations. Compressibility parameters, such as isothermal compressibility, provide information about the reactivity of pharmaceuticals and ionic liquids to pressure changes, which influences their performance under various physiological conditions.

Ionic liquids, with their customizable physical and chemical properties, are a promising medium for drugs solubilization and delivery. Their unique combination of high ionic conductivity, low volatility, and thermal stability improves drug solubility and permeability, providing a diverse platform for therapeutic development. The combination of volumetric and compressibility data helps to optimize the physicochemical parameters of drug-ionic liquid systems, resulting in controlled release and targeted distribution. This study emphasizes the significance of these features in the pharmaceutical industry and ionic liquids' potential as a transformational component in drugs development.

**References**

1. A. Jain, A. S. Chandak, S. P. Zodape, J. Chem. Eng. Data, 69(2024) 59–72.
2. A.S. Chandak, A. Jain, S.P. Zodape, J. Mol. Liq. 383 (2023) 122100.
3. A. Jain, S.P. Zodape, J. Mol. Liq.363 (2022) 119817.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Fundamentals and Applications of Aqueous Biphasic Systems Composed of Deep Eutectic Solvent

**Sushma P. Ijardar**

Department of Chemistry, Veer Narmad South Gujarat University, Surat 395007, India

**Keywords**: aqueous biphasic systems, deep eutectic solvent, extraction

Aqueous biphasic systems (ABSs) were put forward as a suitable and sustainable replacement for traditional liquid-liquid extraction (LLE) used for the isolation, purification, and separation of biological substances. ABSs mainly composed of a large amount of water, need shorter equilibration time and potential scale-up from laboratory to industry. The aqueous solutions of two solutes with opposite polarities at a particular temperature, pH, and concentration resulted in the formation of ABSs [1]. Earlier, polymer-based ABSs were regarded as reliable and sustainable systems for separation purposes [2]. In the early 2000s, novel ABSs was developed by incorporating ILs as phase-forming components to broaden the scope of applications of the ABSs [3]. Recently, Deep Eutectic solvents have been introduced as a new class of green solvents, capable of replacing traditional volatile organic solvents (VOSs) in industry. DESs can be prepared using several other combinations of HBA: HBD, hence, easy to alter the polarity of phases and promote ABS formation [4]. ABS composed of quaternary ammonium salt based DESs and potassium inorganic salts are discussed. The various factors responsible for formation of ABS of DES are discussed. The applicability of ABSs was investigated for the separation of watersoluble dyes [5]. The developed systems would contribute immensely to environmental sustainability as one of the millennial development goals (MDGs).

## References

[1] M.G. Freire, Ionic-liquid-based aqueous biphasic systems: fundamentals and applications, Berlin Heidelberg: *Springer*; 2016.
[2] E.A. Oke, S.P. Ijardar, *J. Mol. Liq.* 334 (**2021**) 116027.
[3] E.A. Oke, S.P. Ijardar, *Separ. Sci. Technol.* 58 (**2023**) 2463–2481.
[4] E.A. Oke, S.P. Ijardar, *Biochem. Eng.* J. 176 (**2021**) 108211.
[5] E.A. Oke, S.P. *J. Mol. Liq.* 375 (**2023**) 121372.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermodynamics and Wetting of Aqueous Solutions of Benign Solvents

**VICKRAMJEET SINGH**

Department of Chemistry, Dr. B. R. Ambedkar National Institute of Technology, Jalandhar 144008, Punjab, India.
*Corresponding author: singhvj@nitj.ac.in

**Keywords**: Ionic liquids, wetting, thermodynamics, drop motion

Ionic liquids (ILs), a novel class of designer solvents, have been used in numerous applications, including biphasic separation technologies, electroplating, drug delivery, lubrication, $CO_2$ capture, and as solvents for synthesis. ILs are synthesized by combining appropriate organic cations and inorganic anions. Protic ionic liquids (PILs), which contain a labile proton, can be easily synthesized through acid-base neutralization. To enhance their applications, ILs are often mixed with various solvents, particularly water. Water acts as a mediator solvent, enhancing the mutual solubility of alcohols and ILs and influencing gas solubilization in aqueous IL mixtures. To overcome the limitation of toxicity related to IL, recently eutectic mixtures have been studied called as deep eutectic solvents (DES). Understanding the nature of interactions between benign solvents, water and typical surfaces is required for the effective application designer solvents. These interactions can significantly impact the applicability of aqueous systems. Despite the rapid growth in the synthesis of new solvent classes due to numerous cation-anion, or hydrogen bond donor-acceptor combinations, there remains a lack of experimental thermodynamic and wetting data. This study evaluates and discusses the physicochemical and interfacial properties of aqueous solutions of benign solvents.

18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024

# Influence of environment friendly solvents and polymers upon the chemical and surface properties surface active agents for their industrial applications

**ASHWANI KUMAR SOOD**[1*]

[1]*Department of Chemistry, Guru Nanak Dev University, Amritsar-143005
*Email: aksoodchem@yahoo.co.in

**Keywords**: surfactant, critical micelle concentration, co-solvents, micellar parameters

The chemical, micellar and surface characteristics of Surface-Active Agents (surfactants) are considerably significant due to their applications in industrial, pharmaceutical, drug delivery and largely rely on the solvent system in which they are utilized. Therefore, various additives as well as solvents, polymers are incorporated to the surfactant preparations to improve their surface features. Addition of solvents to the surfactant solutions bring out many changes in the micellar behaviour, which mainly occurs due to some modifications in the solvent structure and surfactant aggregates. The development of micelle mostly relies on the hydrophobic nature of surfactants as well as solvent. Due to this, it is very significant to analyse the role played by solvent media in order to figure out the micellization phenomenon. The unremitting interest in mixed surfactants also stems from their tendency to efficiently solubilize hydrophobic compounds. This property is due to their synergistic behaviour and has been exploited in numerous industrial applications to optimize performance, minimize the surfactant requirement, and minimize the consequent negative impact on the environment. These mixtures are, therefore, being widely used in cleansing formulations, in synthesis of nanostructure materials and pharmaceutics, etc. In view of their enormous fundamental and commercial importance, the study of mixed surfactant systems has become a topic of pursuit for scientists.

**References**

[1] A. K. Sood, S. K. Godara, M. A. *Tenside Surfact. Det.* 61(**2024**), 54-62
[2] H. Singh, T. Raj, A. K. Sood, T. S. Banipal, *ChemistrySelect* 9 (**2024**) e202304708.
[3] O. Sethi, M. Singh, A. K. Sood, T. S. Kang, *ChemphysChem* 24 (**2023**) e202300293.

# Thermophysical and FTIR properties of protein model compounds in aqueous Ionic Liquid solutions

**P. PATYAR**[1]*

[1]Department of Chemistry, Punjabi University, Patiala, 147 002, Punjab, India
*Corresponding author: poonam_chem@yahoo.co.in; poonampatyar@pbi.ac.in

**Keywords**: Ionic Liquids, Amino Acids, Density, Viscosity, FTIR, 1-butyl-3-methylimidazolium bromide

Amino acids, as fundamental structural units of peptides and proteins, play an essential role in biological systems, influencing biomolecule solubility, denaturation, and activity [1-3]. The investigation of such effects on the thermophysical properties of model compounds in the presence of electrolyte solutions provides insight into solute-solvent and solute-solute interactions on biomolecules [4-5]. Ionic liquids (ILs) as organic electrolytes and green solvents are composed of an organic cation and an inorganic anion liquid at ambient conditions. In the past decade, extensive investigations showed that using ILs as reaction media for processes involving biologically relevant compounds is promising because of their successful application in kinetic resolution, biocatalysis, biosynthesis, separation and purification processes [6]. The scope of this information helps investigate the interactions of amino acids in ILs. To accomplish this goal, the densities $(\rho)$, viscosities $(\eta)$ and FTIR studies of glycine, L-alanine, L-serine, L-threonine, and DL-$\alpha$-aminobutyric acid in aqueous 1-butyl-3-methylimidazolium bromide, $[BMIm][Br]$ solutions of different molalities were determined over the temperature range $T$ = (298.15-318.15) K. Density and viscosity data have been used to calculate various parameters such as apparent molar volumes $(V_{\emptyset})$, partial molar volumes $(V_2^o)$, viscosity $B$-coefficients, temperature coefficients $(\mathrm{d}B/dT)$, transfer parameters, *i.e.,* $\Delta_{tr}V_2^o$and $\Delta_{tr}B$, interaction parameters, $Y_{AB}$ and $Y_{ABB}$ and hydration number, *i.e.* $n_H$ and $N_h$. Also, partial molar expansibilities $(\partial V_2^o/\partial T)_P$, their second-order derivatives $(\partial^2 V_2^o/\partial T^2)_P$, and isobaric thermal expansion coefficients $(\alpha_{IL})$ were calculated. The charged end groups, $D\ (-NH_3^+,\ -COO^-)$ and side-chain contributions of the amino acids, $D(-R)$, have also been obtained from $V_2^o$and viscosity $B$-coefficients data. Results obtained have been interpreted in terms of amino acids + water + $[BMIm][Br]$ interactions. FTIR data has been interpreted to study the interactions between amino acids and aqueous$[BMIm][Br]$ solutions.

***References:***
[1] T. Banerjee, N. Kishore, Journal of Solution Chemistry, 34 (**2005)** 2745-2748.
[2] A. Ali, S. Khan, S. Hyder, Journal of Chemical Thermodynamics, 39 (**2007)** 613-620.
[3] Z. Yan, J. Wang, W. Kong, Fluid Phase Equilibria, 215 (**2014)**143-150.
[4] R. Badarayani, A. Kumar, Journal of Chemical Thermodynamics 36 (**2004**) 49-58.
[5] J. Wang, Z Yan, K. Zhuo, J. Lu, Biophysical Chemistry 80 (**1999)** 179-188.
[6] Z. Yan, R. Geng, B. Gu, Q. Pan, J. Wang, Fluid Phase Equilibria 367 (**2014)** 125-134.

T10- IL 54

# Green Solvents of the Future: Towards a Sustainable alternative

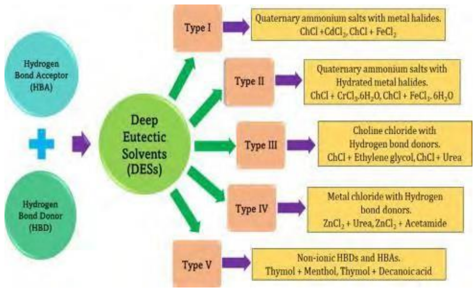
**PROF. RANJAN DEY,** **FRSC, FICS, MNASc.**[1]*

[1] Dept of Chemistry, BITS PILANI K K BIRLA GOA CAMPUS, ZUARINAGAR, GOA, INDIA.
*Corresponding author: e-mail: ranjandey@goa.bits-pilani.ac.in

**Keywords**: Industrial Solvents, Green Alternatives, DES

The chemical, pharmaceutical, petrochemical, reservoir engineering, dyes, adhesives and allied industries are completely dependent on the usage of industrial solvents like DMSO, NMP, DMF, etc., and a vast majority of them are Volatile Organic Compounds (VOCs) imbued with high degree of toxicity and volatility whose usage leads to very serious and irreparable environmental hazards. Millions of people encounter these solvents directly or indirectly through various means. A vast majority of these solvents are known carcinogenic and mutagenic [1]. It is imperative to develop newer, sustainable, cost effective and less energy intensive green technologies to carry out the industrial solvent – water separation.

This talk will delve upon these green alternatives and their applications in multifarious industrial applications. These will include Deep Eutectic Solvents and usage of encapsulated phase change materials (PCM) based magnetic nanoparticles [2]. A part of the Talk will also involve the usage and application of AI-ML based algorithms to predict thermophysical properties [3] and how they can also be used to optimize and classify the best solvent to be used for extraction and carry out a suitable post-hoc analysis to identify which of these properties are most important for the separation.



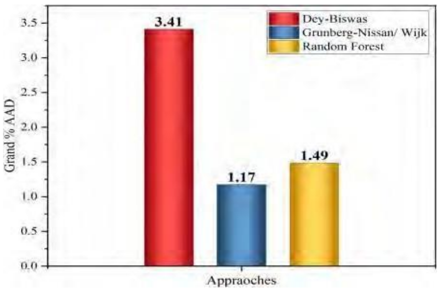


**Fig 1** **Fig 2**

**Fig. 1 Types of deep eutectic solvents, *Journal of Molecular Liquids, 379 (2023) 12176.***
**Fig. 2 Comparison of Grand %AAD, *Journal of Molecular Liquids, 397 (2024) 124147.***

**References**
[1] Aditi Prabhune, Ranjan Dey, *Journal of Molecular Liquids 379 (2023) 121676.*
[2] S. Bhattacharya *et al*, *Sustainable Energy Technologies and Assessments,57( 2023) 103194.*
[3] A. Prabhune, A. Mathur, S. Saha, R. Dey, *Journal of Molecular Liquids 397 (2024) 124147.*

**T10- IL 55**

# Correlation between crystal structure parameters with optical, electronic, luminescent, and magnetic parameters of barium hexaferrite nanomaterials at controlled thermal temperature

**ZEESHAN HASMI[1], RAKESH KUMAR SINGH[1], NISHANT KUMAR[1], MONALISA[1],
R. K. VERMA[2,3,4]**

[1]Aryabhatta Knowledge University, Patna: 800001
[2] University Department of Chemistry, Magadh University, Bodh Gaya 824234, India
[3] Patna University, Patna-800005
[4] Munger University, Munger-811201
*Corresponding author: e-mail: rakeshsinghpu@gmail.com

**Keywords**: thermal analysis, DSC, citrate precursor, optical properties

The citrate precursor sol-gel method is used to create M-type barium hexaferrite ($BaFe_{12}O_{19}$)[1]. Our earlier report has been revisited with extra inputs. The hexagonal crystal structure with P63/mmc space group of the synthesized nanomaterials was confirmed by the X-ray spectra and was found to be present in a pure phase. In the hexaferrite nanomaterials, the crystallite size and lattice strain are determined using the Williamson-Hall plot. Due to induced lattice strains in the samples, the lattice parameters (a) and (c) exhibit considerable increases. The FTIR spectrum effectively supports the XRD findings. The direct and indirect band was found to decrease from 2.32 eV to 1.81 eV and 3.41 eV to 3.18 eV respectively. Zeta potential measurements show that the stability increases with the annealing temperature. With annealing, the magnetic properties of nanomaterials are improved, with notable rise in magnetization (26.91-71.74 emu/g) and retentivity (37.24-72.25 emu/g). Coercivity dramatically rises from 161.33 to 4563 Gauss. The present study investigates the relationship between induced lattice strain and enrichment of structural, optical and magnetic characteristics at various annealing temperatures

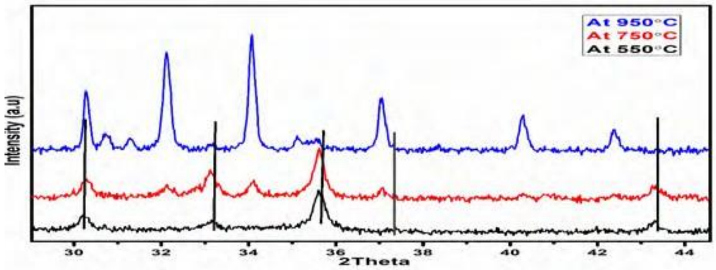
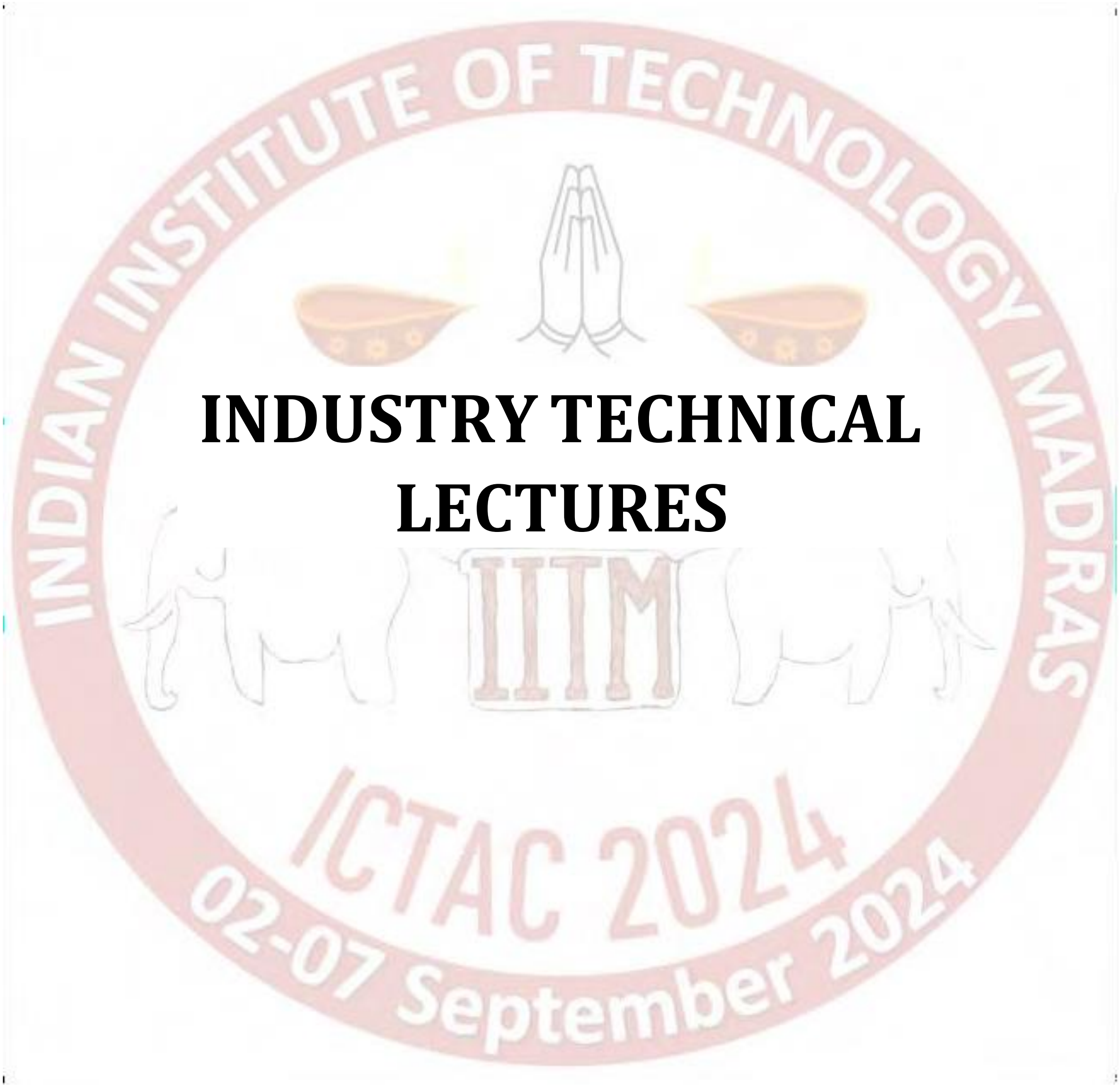


Fig. 1 : Shift in prominent peak and planes [104] and [108] intensity of intermediate phases (-Fe2O3) with annealing temperature

## References

[1] R. K. Verma, R. K. Singh, A. Narayan, L. Verma, A.K. Singh, A. Kumar, P.K. Pathak, A. K. Aman. Low-temperature synthesis of hexagonal barium ferrite (BaFe12O19) nanoparticles by annealing at 450 °C followed by quenching. J Therm Anal Calorim.2017;129: 691–9.



# INDUSTRY TECHNICAL LECTURES

**IS 01**

# Simultaneous thermal analysis - mass spectrometry system with two types of interface structures and its applications

**TADASHI ARII**

Thermal Analysis, Product Division, Rigaku Corporation, 3-9-12 Matsubara,
Akishima, Tokyo 196-8666, Japan
Corresponding author: e-mail: t-arii@rigaku.co.jp

**Keywords**: TG-DTA-MS, Skimmer, Capillary, Bisphenol A

During recent years, TG-DTA-MS which combines Simultaneous Thermal Analysis (STA/TG-DTA) and Mass spectrometry (MS), has been utilized in a wide range of applications as a method of hyphenated simultaneous thermal analysis. We have been developed and proposed Thermo Mass Photo (TG-DTA-MS) equipped with both soft ionization and skimmer interface technologies, which is the powerful tool for MS analysis.[1-2] TG-DTA-MS requires a gas transport interface system that significantly affects the performance for accurately introducing the gases evolved from the sample in the TG-DTA into the MS, and two typical types have been proposed: capillary and skimmer interface types.

In this study, we have developed a new capillary interface that minimises the cold point of the gas interface pathway to allow the introduction of high boiling point gas component species close to the MS ionisation source, building the Thermo Mass Photo that combines the complementary features of both the skimmer and the capillary interface.

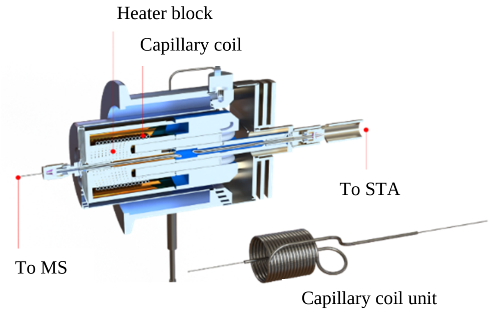


Fig. 1 : Cross-sectional view of new capillary interface

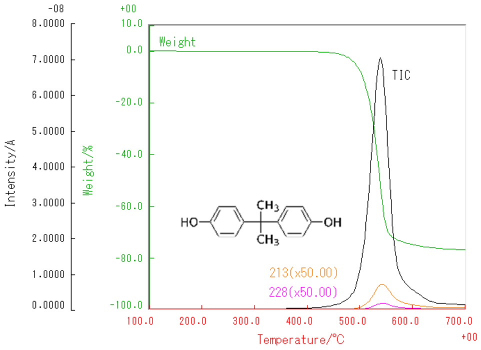


Fig. 2 : TG-MS results in helium atmosphere for polycarbonate.

The TG-MS results of 2mg of polycarbonate heated up to 700°C at 20°C/min in He are shown in Fig. 2. The *m/z* 213 and 228 ion peaks are clearly detected, revealing that bisphenol A, BPA is evolved during the pyrolysis of polycarbonate (500-600°C).

**References**
[1] T. Arii, K. Motomura and S. Otake, *J. Mass Spectrom. Soc. Jpn.*, 59 (2011) 5.
[2] L. L. Celiz and T. Arii, *J Therm Anal Calorim.*, 116 (2014) 1435.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Unveil the new Pyris-9 with the Power of Hyphenation

**Dr. Manohar Rao**

Global Product Line Leader PerkinElmer INDIA & South Asia
*Corresponding author: India.Customercare@perkinelmer.com

The talk will cover the unveiling of new Pyris™ TGA 9, DSC 9, and STA 9 systems: a new generation of compact, durable, high-resolution, and low-maintenance thermal analysis systems with our groundbreaking interchangeable furnace design enhancing versatility & productivity. With focus on unique PerkinElmer Hyphenation System, a modular, multimodal TGA, IR, and GC/MS solution managed by an electronic control panel, enabling complete sample characterization with minimal sample prep. Using the power of hyphenation focus on new relevant application like Polymer recycling and Microplastics.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermal Conductivity Assessment: An Innovative Approach

**G. Padmanabhan ***

Vice President
LCGC Bioanalytical Solutions
*Corresponding author: e-mail: padmanabhan@lcgcindia.com

**Keywords:** Thermal Conductivity, Effusivity

As the importance of material characterization continues to rise, accurately assessing material properties becomes increasingly vital for understanding and optimizing performance. Among these properties, thermal conductivity is particularly crucial. However, its evaluation presents several challenges, often influenced by factors such as sample type, dimensions, and compatibility. C-Therm, the global leader in thermal conductivity instrumentation for the testing and measurement of polymers, ceramics, composites, insulation, textiles, and a wide range of other materials, has pioneered innovative solutions to overcome these challenges. By delivering valuable insights into properties like thermal diffusivity, conductivity, and Effusivity, C-Therm is driving advancements that are significantly benefiting the scientific community. This paper and presentation will delve into the transient method, which employs a variety of sensors specifically designed for different materials, enabling precise thermal conductivity assessments. Additionally, it will compare the various techniques available to users, with the goal of sparking discussions on future developments in the field.

# RSC India Activities and Membership Benefits

**Rajdip Roy ***

Membership Executive - External Relationships Royal Chemistry India Private Limited
A subsidiary of The Royal Society of Chemistry The Regus, Unit No. 2201A, 22nd Floor, World
Trade Centre Brigade Gateway Campus, 26/1, Dr. Rajkumar Road Malleswaram, Bangalore -
560055, Karnataka, India *Corresponding
author: e-mail: www.rsc.org

The Royal Society of Chemistry (RSC) is a learned society with the goal of "advancing the chemical sciences" in our day-to-day life keeping in mind the importance of chemistry in our society. RSC provides a unique platform to connect students, teachers, researchers, scientists together for the development and recognition of professional capabilities and to publish new cutting-edge research. Being an UK organization, with the headquarters located in Cambridge and London, RSC has now extended its global offices to all over the world and since 2010, RSC India office has been actively operating from Bengaluru. With more than 2,500 members and 2nd highest article submissions & articles published across all RSC journals in 2023 from India, RSC India is also constantly trying to engage the chemical community here in India with social, educational outreach activities and membership benefits in India specific way.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Advanced Thermal Analysis Techniques for the Characterization of Sustainable Polymers

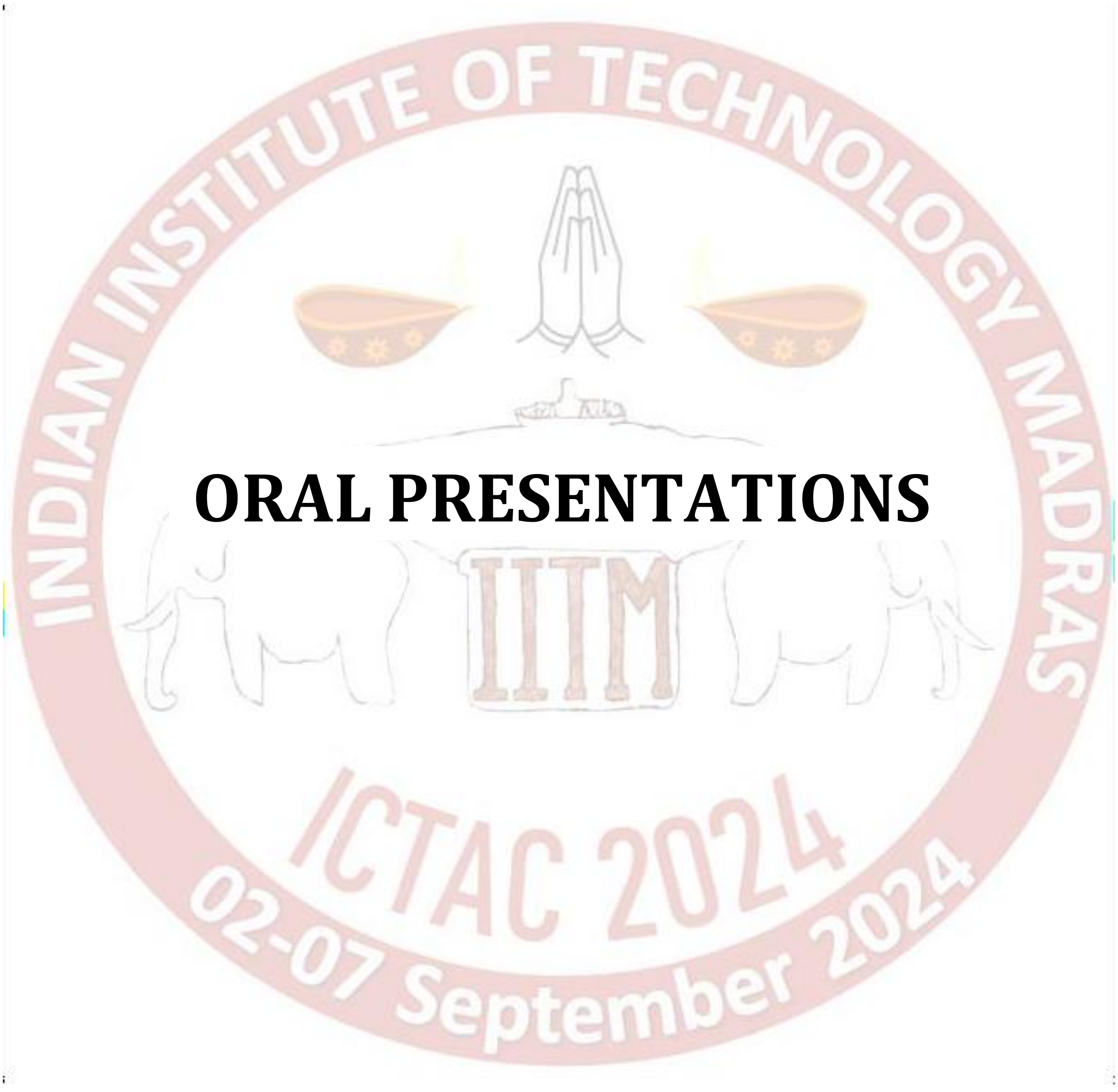
**RAJ GANESH JEGADEESAN** *

TA Instruments Division- Waters LLC, Bangalore, India
Email: j_rajganesh@waters.com

**Keywords**: polymer, biopolymers, recycled polymers, DSC, TGA, Polymer testing, thermal analysis, sustainable materials

Demand from consumers, brand owners, and public policy are driving a need for sustainability in plastics, affecting companies at every stage of plastics production. In response, the plastics industry is tackling the problem of plastics waste through a wide range of sustainable solutions including the use of post-consumer recycled (PCR) and post-industrial recycled (PIR) resins, bio-sourced/ bio-degradable polymers, and the development of new and innovative polymers. Thermal analysis solutions from TA Instruments- Waters LLC enable R&D scientists and process engineers to characterize complex recycled resin feedstocks more effectively and explore their impact on their products and processes while improving the operational efficiency of their analytical laboratories. For sustainable polymers, one of the biggest challenges is determining how post-consumer recycled materials differ in their physical properties from traditional virgin resin. The polymer characterization technique such as TGA, DSC, and DMA/TMA analysis can help with this challenge by screening and understanding the behaviours and properties of such materials. In turn, the results can predict any adverse product performance effects from the use of recycled materials and lead to improvements in the design of new renewably sourced or bio-degradable polymer candidates. These material characterization helps research scientists; process engineers and QA/QC analysts gain insights into their material and answer important questions as they innovate to make plastics more sustainable at every step of the value chain.

# ORAL PRESENTATIONS



*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# The study of carbon-epoxy laminate with novel flame retardants by cone calorimetry

**ANNA VYKYDALOVÁ[1,2,3]*, ANITA ECKSTEIN[1], ZDENKO ŠPITÁLSKÝ[1]**

[1] Polymer Institute, Slovak Academy of Sciences, Dúbravská cesta 9, 845 41 Bratislava, Slovakia
[2] Faculty of Chemical and Food Technology, Slovak University of Technology, Radlinského 9
812 37 Bratislava, Slovakia
[3] Institute of Inorganic Chemistry, Czech Academy of Sciences, Husinec-Řež 1001, 250 68 Řež, Czech Republic
*Corresponding author: anna.vykydalova@savba.sk

**Keywords**: epoxide, flame retardants, cone calorimetry, fire testing

Epoxides are highly reactive cyclic ethers which are used in specialized fields (manufacture of coatings, adhesives, plastics and materials for building and construction applications, etc.). These materials are highly flammable and for this reason the addition of flame retardants is desirable. In general, flame retardants are usually added to materials such as plastics, coatings, textiles, building materials and other products [1]. A variety of different chemicals, with different properties and structures, act as flame retardants, and these chemicals are often combined for improved their effectiveness. Flame retardants are able to slow down the spread of fire or even prevent the initial ignition [2]. For these reasons the development and study of new FRs are necessary.

In this study a new flame retardants had been developed and tested by cone calorimetry. FRs were added to the epoxide matrix to improve their thermal and flame retardant properties. The meaning was to compare the influence of the new flame retardants (less toxicity). The goal is to extend the area of carbon-epoxy laminates applications, especially to transportation (railways, automotive or aviation) and construction industry. The novel FRs which containing amine groups and phosphazenes are covalently bound to the matrix. The difference in mixing the flame retardant into the matrix were also tried. It seems that the way of mixing the materials can have an influence on flammability. The results have shown that these flame retardants are a promising alternative to currently used products.

Acknowledgements: The authors appreciate the financial support from the Slovak grant agency VEGA (Grants No 2/0137/23).

**References**

[1] Sienel G., Rieth R, Rowbottom K.T.: *Epoxides. In: Ullmann's Encyclopedia of Industrial Chemistry*. John Wiley, New York, 2000.
[2] L.A. Hollingbery, T.R. Hull, *Thermochim. Acta* 509 (2010) 1.

**T1- OP 02**

# Phase Equilibria and of Structure II Clathrate Hydrate Formed with $CO_2$+Cyclohexanone

LEO KAMIYA[1], RYONOSUKE KASAI[1], SATOSHI TAKEYA[2], RYO OHMURA[1]*

[1]Department of Mechanical Engineering, Keio University, Yokohama 223-8522, Japan

[2]National Institute of Advanced Industrial Science and Technology (AIST), Central 5, 1-1-1 Higashi, Tsukuba 305-8565, Japan.

**Keywords**: phase equilibria, powder Xray diffraction, clathrate hydrate

This study presents the phase equilibrium and crystallographic data of the hydrate formed in the $CO_2$ + cyclohexanone + water system. The phase equilibrium conditions were measured and powder X-ray diffraction measurements were conducted. The formation of the structure II hydrate in the system of cyclohexanone + water + $CO_2$ was observed at temperatures ranging from 270.0 K to 275.6 K and pressures from 0.623 MPa to 1.703 MPa.

At temperatures between 270.0 K and 275.6 K and pressures between 0.623 MPa and 1.703 MPa, the structure II hydrate was observed to form, and the phase equilibrium condition was alleviated in the system of $CO_2$ + cyclohexanone + water, while the hydrate formed at 276.5 K - 280.7 K and 2.021 MPa – 3.330 MPa, formed structure I, and cyclohexanone acted as an inhibitor. The equilibrium conditions were measured with the isochoric method, revealing different slopes at high and low temperatures. The high-temperature slope closely resembled the one previously reported data of structure I. Throughout the structural phase transition, temperature and pressure were continuously monitored, resulting in a slope change. To directly determine the hydrate structure, PXRD measurements were conducted on two samples: one from the high-temperature side and the other from the low-temperature side. The sample from the high-temperature side exhibited structure I with a lattice constant of 11.8749 (9) Å at 153 K, while the low-temperature sample displayed structure II with a lattice constant of 17.443(1) Å at 153 K.

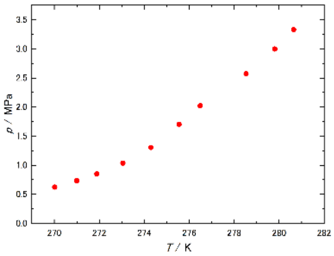


Fig. 1: Hydrate phase equilibrium diagram of $CO_2$ + cyclohexanone + water system

**References**

[1] T.A. Strobel, K.C. Hester, E.D. Sloan, C.A. Koh, J Am Chem Soc 129 (2007) 9544–9545.
[2] S.H. Khudaida, P.Y. Lin, C.S. Su, J Chem Eng Data 68 (2023) 2087–2095.
[3] R. Ohmura, S. Takeya, T. Uchida, I.Y. Ikeda, T. Ebinuma, H. Narita, Fluid Phase Equilib 221 (2004)

# Thermal Analysis and Calorimetric Comparison of Taiwanese Solid Recovered Fuels Across Seasonal Variations

Yu-Cheng Lin[1], Wei-Cheng Lin[2], Yi-Chun Yu[3], Chen-Rui Cao[4], Chi-Min Shu[2,3,*]

[1] Department of Safety, Health, and Environmental Engineering, YunTech, 123, University Rd., Sec. 3, Douliou, Yunlin 64002, Taiwan, ROC
[2] Centre for Process Safety and Industrial Disaster Prevention, YunTech, 123, University Rd., Sec. 3, Douliou, Yunlin 64002, Taiwan, ROC
[3] Department and Graduate School of Safety, Health, and Environmental Engineering, YunTech., 123, University Rd., Sec. 3, Douliou, Yunlin, 64002, Taiwan, ROC
[4] Graduate School of Engineering Science and Technology, National Yunlin University of Science and Technology, YunTech., 123, University Rd., Sec. 3, Douliou, Yunlin, 64002, Taiwan, ROC
*Corresponding author: e-mail: shucm@yuntech.edu.tw

**Keywords**: Boron-containing based ILs, Flame retardancy, Combustion, Phosphorus-containing based ILs, Fire protection

This study investigated the effects of incorporating phosphorus-containing based and boron-based ionic liquids (ILs), including 1-butyl-3-methylimidazolium dibutyl phosphate ([Bmim][DBP]), 1-butyl-3-methylimidazolium hexafluorophosphate ([Bmim][PF$_6$]), and 1-butyl-3-methylimidazolium acetate ([Bmim][BF$_4$]), on the flame retardancy and thermal stability of cutting oils and engine oils. These findings suggest that boron-based ILs could enhance hightemperature resistance and reduce heat release during combustion. Phosphorus-containing based ILs could form a protective carbon layer, thereby improving fire protection. Additionally, different ILs had varying effects on exothermic changes and thermal stability in industrial oils, with [Bmim][DBP] showing the most significant improvement.

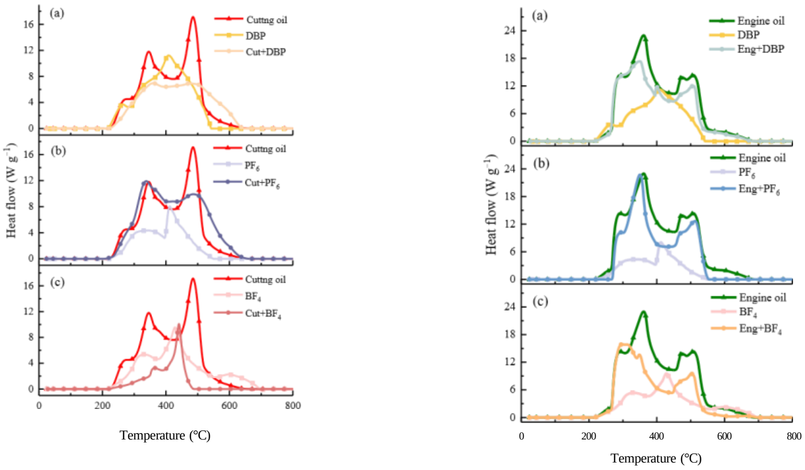


Fig. 1 : Heat flow versus temperature diagram of ILs, cutting, engine oils, and blended oils (a) [Bmim][DBP], (b) [Bmim][PF$_6$], (c) [Bmim][BF$_4$].

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Advancements in Heat Transfer: Metal-Foam Tube Banks for Compact Refrigeration Systems

**ANIKET A. DHAVALE[1]*, DR. MANDAR M.LELE[2]**

[1]Savitribai Phule Pune University, Department of Technology, Pune 411007, India
[2] School of Mechanical Engineering, MIT World Peace University, Pune 411038, India

*Corresponding author: aniket.dhavale83@gmail.com

**Keywords**: metal foam, heat transfer, evaporators, simulation

Traditional evaporator designs are often bulky and heavy, limiting their use in compact or mobile refrigeration systems. Improving energy efficiency in refrigeration is crucial for reducing operational costs and environmental impact. Open-cell metal foam, with its high surface area-to-volume ratio and excellent thermal conductivity, offers a promising solution. This study investigates the feasibility of using metal foam structures in evaporators to enhance efficiency and performance in compact refrigeration systems. In this paper, the heat transfer enhancement of forced convection in metal foam-wrapped tube banks is studied through simulation using ANSYS-Fluent 2021R2. The Darcy-Forchheimer-Brinkman momentum model, considering viscous loss and inertial loss, and the local thermal non-equilibrium energy model, which considers the interstitial heat transfer between fluid and solid, are employed for the porous zone. Effects of foam thickness and free stream velocity are analyzed to examine the heat transfer and pressure drop characteristics. Overall, the heat transfer capability of metal foam heat exchangers can surpass conventional compact heat exchangers given an optimal scenario. In an array with fixed foam thickness, better heat transfer performance is obtained at lower free stream velocities. It was also found that, within the designated fluid velocity range, tube banks with thicker foam layers exhibit higher heat transfer rates and larger pressure drops. However, there exists an optimal dimensionless thickness of foam layer that gives the highest area goodness factor for the configuration considered in this study. These findings highlight the potential of metal foam-wrapped tube banks to significantly improve the efficiency and performance of evaporators in compact refrigeration systems.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Comparative Numerical Analysis of Thermal Performance of various Cylindrical Li-ion Cells used in Electric Vehicle Battery Pack with Air, PCM and PCM-Fin-Based Cooling

**DURGESH SRIVASTAV*, NAGESH D. PATIL, PRAVESH CHANDRA SHUKLA**

Indian Institute of Technology Bhilai
*Corresponding author: e-mail: durgeshsr@iitbhilai.ac.in

**Keywords**: Electric Vehicle (EV), Li-ion Battery, Phase Change Material (PCM), Thermal analysis

The world is leading towards decarbonization and greener transportation options. In this regard Electric vehicles (EV) are gaining popularity because of their unique feature of zero tailpipe emission which leads to reduction in urban pollution. Thermal runaway is one of the major challenges associated with EV operation. EVs are powered by Lithium-ion (Li-ion) cells and during the discharging of Li-ion cells, they generate a significant amount of heat, this heat needs to be liberated intime to prevent thermal runaway. In the market, there are several Li-ion cells of different geometry; however, cylindrical cells are the preferred choice for EV application also there are several chemistries but LFP (Lithium iron Phosphate) is preferred choice and its demand is around 40% in 2023 worldwide for EV application [1]. This study focuses on comparative numerical analysis of the surface temperature growth and thermal performance testing of LFP Li-ion cells of various dimensions (18650 26650, and 21700) under the condition of natural air, PCM and PCM-Fin based cooling. It has been observed from previous study that PCM can reduce the temperature of Li-ion cell by 12 °C [2]. In this study MSMD-NTGK Battery Module in Ansys fluent is used for numerical analysis, this model considers both the electric and chemical (entropic) heat generation phenomenon of Li-ion cell during discharging. This study will quantify the thermal management efficiency of PCM and PCM-Fin in these cell geometries as well as this study will provide information about the temperature variation of cell surface at various loads (C-Rates) with respect to time. Which subsequently help in choosing the right cell with suitable cooling system for the right EV Battery pack application.

## *References*

[1] IEA (2024), Global EV Outlook 2024, IEA, Paris https://www.iea.org/reports/global-ev-outlook-2024, Licence: CC BY 4.0

[2] Kizilel, Riza, Rami Sabbah, J. Robert Selman, and Said Al-Hallaj. "An alternative cooling system to enhance the safety of Li-ion battery packs." Journal of Power Sources 194, no. 2 (2009): 1105-1112.

# Characterization of the hydrate formed in the water + ethanol + carbon dioxide system.

## Abstract for ICTAC 2024

**M SATOH[1]*, L KAMIYA. S. TAKEYA[2], R OHMURA,**

[1]Keio university
[2] AIST,
*Author: e-mail: mitsuru122000@gmail.com

**Keywords**: Crystal structure, powder X-ray diffraction, clathrate hydrate

Hydrate formed with the ethanol aqueous solution and gaseous CO2 was characterized by means of powder X-ray diffraction (PXRD) measurements. Crystallographic structure of the hydrate was directly identified. Approximately 40 g of solid hydrate sample was prepared with 50 mass% ethanol solution pressurized with $CO_2$ at 2.2 MPa and 266 K. The hydrate sample was formed with high pressure reactor. The sample was taken out of the reactor at the liquid nitrogen temperature and then subjected to the PXRD measurements. The obtained PXRD profile is shown in Figure 1.

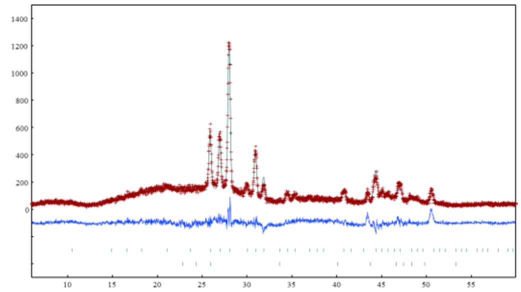


Fig. 1 : PXRD profile of $CO_2$ hydrate formed with ethanol solution

Figure 1 shows that the lattice constant is 11.902 Å at 123 K. This value is significantly greater than those of simple structure I $CO_2$ hydrate, 11.84 Å and $CO_2$ + ethanol hydrate formed from ice and ethanol, 11.88 Å at the same temperature. [1] These results indicate that the crystallographic structure of the three hydrate is common, structure I, but the lattice constant is clearly different. The greater lattice constant of the hydrate formed in this study may indicate the inclusion of greater amount of ethanol molecules in the structure I hydrate. Based on the comparison of the experimental data of the lattice constant and the relevant molecular dynamics analysis, it is inferred that the 50% of the large cage ($5^{12}6^{2}$) of structure I hydrate would be occupied by ethanol molecules. [2]

**References**

[1] Takeshi Makiya, Takashi Murakami, Satoshi Takeya, Amadeu K. Sum, Saman Alavi and Ryo Ohmura. *Physical Chemistry Chemical Physics,* 12.9927-9932, 2010.

[2] Saman Alavi; Satoshi Takeya; Ryo Ohmura; Tom K. Woo; John A. Ripmeester. *J. Chem. Phys.* 133, 2010

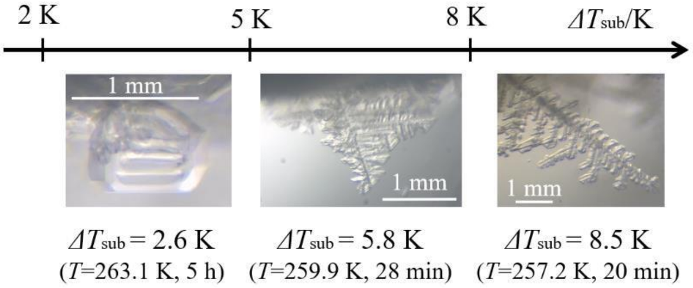
# Crystal Growth and Morphology of $CO_2$ Hydrate with Sodium Chloride Aqueous Solution

**RYONOSUKE KASAI[1], LEO KAMIYA[1], RYO OHMURA[1]***

[1]Department of Mechanical Engineering, Keio University, Yokohama 223-8522, Japan
*Corresponding author: e-mail: rohmura@mech.keio.ac.jp

**Keywords**: clathrate hydrate, desalination, crystal growth, crystal morphology

Crystal growth and morphology of $CO_2$ hydrate in sodium chloride aqueous solution were visually investigated. Clathrate hydrates (hereafter hydrates) are crystalline compounds which are composed of water and guest molecules under low temperature and high-pressure conditions. Guest molecules are encapsuled in cage-like structures made up of hydrogen-bonded water molecules. Clathrate-hydrate-based desalination has been proposed as a novel technology. It is performed by reacting seawater and guest compounds to form hydrates and obtaining fresh water by decomposing hydrates. When this methodology expands to an industrial-scale, mechanical properties of hydrates affects the overall efficiency. Thus, understanding individual crystal growth and crystal morphology of hydrates is essencial. Ohmura et al. reported that there are correlations between crystal morphology of hydrates and subcooling temperature $\Delta T_{\mathrm{sub}}$. $\Delta T_{\mathrm{sub}}$ is defined as the difference between the equilibrium temperature and system temperature. In this study, we observed crystal growth and morphology of $CO_2$ hydrates in NaCl solution (0.20 mass fraction 20 mass%) + $CO_2$ system with changing subcooling temperature from 2.6 K to 8.5 K at 2.1 MPa.



$\Delta T_{\mathrm{sub}} = 2.6$ K ($T$=263.1 K, 5 h) $\Delta T_{\mathrm{sub}} = 5.8$ K ($T$=259.9 K, 28 min) $\Delta T_{\mathrm{sub}} = 8.5$ K ($T$=257.2 K, 20 min)

Fig. 1 : The relationship between $\Delta T_{\mathrm{sub}}$ and crystal morphology

In all experiments, the initial hydrate formation occurred at gas-liquid interface. Fig.1 shows the relationship between $\Delta T_{\mathrm{sub}}$ and crystal morphology. When $\Delta T_{\mathrm{sub}}$ = 2.2 K, hydrates formed polyhedral crystals. $\Delta T_{\mathrm{sub}}$ = 8.2 K, dendritic crystals were observed. $\Delta T_{\mathrm{sub}}$ = 5.5 K, crystals that looks like a combination of polyhedral and dendritic structure was observed. The relation of $\Delta T_{\mathrm{sub}}$ and crystal morphology was generally the same as in a previous study. However, crystal growth rate was much slower than previous study.

**References**

[1] P. Babu, A. Nambiar, T. He, I. A. Karimi, J. D. Lee, P. Englezos, P. Linga. *ACS Sustainable Chem. Eng*, 6 (**2018)** 8093-8107.

[2] R. Ohmura, W. Shimada, T. Uchida, Y. H. Mori, S. Takeya, J. Nagao, H. Minagawa, T. Ebinuma, H. Narita. *Philosophical Magazine*, 84 **(2004)** 1-16.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermophysical properties of thermal energy storage medium for battery cooling: Thermophysical properties of 2,5-dimethyl-2,5-hexanediol hydrates

**I. MITSUI[1]*, R. OHMURA**

[1]Department of Mechanical Engineering, Keio University, Yokohama 223-8522, Japan

**Keywords**: hydrate, energy storage, phase change materials, phase equilibrium

The renewable energy has the potential to solve environmental problems. The goal of renewable energy is to achieve stable generation and supply. Energy storage system (ESS) enable supply of renewable energy. There are several systems for ESS, of which lithium-ion batteries are the most widespread. However, the weak point of the lithium-ion battery is heating due to charging and discharging. The ideal battery operating temperature is about 40 ℃ . It is necessary to cool the battery and conventional cooling methods include forced convection cooling and water cooling. Using 2,5-dimethyl-2,5-hexanediol (DM-HDO) hydrate as phase change material (PCM) is proposed as a new method. The hydrate has a large dissociation heat and will form and dissociate at approximatery 40 ℃ under atmosphere pressure conditions. Battery cooling which uses DM-HDO hydrate would have enough performance regarding that stability of heat transfer. To adapt DM-HDO to battery cooling, it is necessary to clarify the changes in physical properties as the concentration of the aqueous solution is varied.

In this study, the equilibrium temperature and dissociation heats were measured. The equilibrium temperature was measured by visual observation, the dissociation heats were measured by DSC. The range of aqueous solution concentration was 0.40 to 0.52 in mass fraction. The highest equilibrium temperature was 38.3 ℃, the dissociation heat was 165.3 kJ/kg at the mass fraction of 0.50.

Table 1: The equilibrium temperature and dissociation heat of DM-HDO hydrate

| Mass fraction, $w$ | Equilibrium temperature, $T_{\mathrm{eq}}$ /℃ | Dissociation heat, $\Delta H$ /kJ · kg$^{-1}$ |
|---|---|---|
| 0.41 | 37.6 | 123.2 |
| 0.46 | 38.1 | 146.3 |
| 0.47 | 38.0 | 147.6 |
| 0.50 | 38.3 | 165.3 |

**References**

[1] B. Shabani, M. Biju, *Energies.* 8 (2015) 10153-10177

[2] Goates, J. R., Bevan Ott, J., Woolley, E. M., & Priest, J. G. (1982). *J. Chem. SOC., Faraday Trans.* 1 (Vol. 78).

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermogravimetric analysis of hydrated vanadium oxide nanostructures

**SURESH BANDI[1], AJEET K. SRIVASTAV[2]***

[1]Department of Metallurgical and Materials Engineering, Malaviya National Institute of Technology Jaipur, Jaipur 302017, India
[2]Department of Metallurgical and Materials Engineering, Visvesvaraya National Institute of Technology Nagpur, Nagpur 440010, India

**Keywords**: Hydrated vanadium oxide, Nanostructures, Nonstoichiometry, TGA

Hydrated vanadium oxide nanosheets were synthesized following the chemical co-precipitation approach. Scanning Electron Microscopy and X-ray diffraction analysis were utilized for the phase identification and the morphology evolution. Further, a careful thermogravimetric analysis was employed to deduce the water content and stoichiometry of the synthesized material. We found the stoichiometry of the hydrated vanadium oxide as $(VO)_{0.1}V_2O_5.2.35H_2O$. Interestingly, the initially obtained $(VO)_{0.1}V_2O_5.2.35H_2O$ possesses the enhanced interlayer spacing of 14.6 Å as compared to the 11.5 Å reported for $V_2O_5.1.6H_2O$ xerogels.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Solvation Behavior of Antidepressant Duloxetine Hydrochloride with Aqueous Myo-Inositol and different Amino acids solution

**KOMAL M. JAMKHANDE[1], NIRAJ T. KHATY[2], CHANDRASHEKHAR P. PANDHURNEKAR[3], VIJAY M. TANGDE[1*], SUDHAKAR S. DHONDGE[4]**

1Department of Chemistry, Rashtrasant Tukadoji Maharaj Nagpur University, Nagpur 440033, India
2Department of Chemistry, Laxminarayan Innovation Technological University, Nagpur 440033, India
3Department of Chemistry, Shri Ramdeobaba college of Engineering and Management, Nagpur 440013, India
4P.G. Department of Chemistry, S. K. Porwal College, Kamptee, Nagpur 441001, India
*Corresponding author: vijaytn6@gmail.com

**Keywords**: Density, sound velocity, viscosity, Duloxetine hydrochloride, myo-Inositol

Present study reports the densities ($\rho$), speed of sound ($u$) and viscosities ($\eta$) of Duloxetine hydrochloride in aqueous and aqueous myo-Inositol and different amino acids solution of different molal concentrations at seven temperatures ranging from (288.15 - 318.15) K. Using the corresponding density and speed of sound data, different thermophysical parameters like apparent molar volume ($V_{\emptyset}$), limiting apparent molar volume ($V_{\emptyset}$ ), partial molar volume of transfer ($\Delta\ V_{\emptyset}$ ), thermal expansion coefficient ($\alpha^{*}$), limiting apparent molal expansibilities ($E_{\emptyset}$), isentropic compressibility ($\kappa$ ), apparent molar isentropic compression ($K_{\emptyset}$), limiting apparent molal isentropic compression of solute ($K_{\ ,\emptyset}$), partial molar compression of transfer ($\Delta\ K_{\ ,}$) and hydration number ($n$ ), have been calculated. The viscosity data have been used to determine Falkenhagen coefficient A, Jones-Dole coefficient B on the basis of Jones-Dole equation. By using the Nightingale Benck and Eyring equation the free energy, enthalpy ($\Delta H$ ) and entropy of activation ($\Delta S$ ) were calculated. The solvation behavior of Duloxetine hydrochloride, an antidepressant drug, in aqueous systems have been discussed from the result and various drug molecular interactions have been studied from thermophysical properties[1][2][3]. Since electrolytes are a crucial component of biological systems, studying them can help us better understand how drugs work, which helps us illustrate the relationship between drugs and electrolytes.

## References

[1] P. Y. Umredkar, V. M. Tangde, N. T. Khaty, K. S. Ganorkar, and S. S. Dhondge, "Effect of aqueous solutions of KCl, MgCl2, Dextrose and Urea on solvation behavior of aqueous myo-Inositol," J. Mol. Liq., vol. 377, p. 121522, 2023, doi: 10.1016/j.molliq.2023.121522.

[2] J. C. Thermodynamics, N. G. Sheikh, V. M. Tangde, S. S. Dhondge, A. S. Dhondge, and N. T. Khaty, "Investigation of the effect of temperature on aggregation behaviour and thermodynamic properties of Ornithine monohydrochloride in aqueous and aqueous dextrose and urea solutions," J. Chem. Thermodyn., vol. 151, p. 106254, 2020, doi: 10.1016/j.jct.2020.106254.

[3] Ankita and A. K. Nain, "Volumetric, acoustic and viscometric studies of solute-solute and solute-solvent interactions of isoniazid in aqueous-glucose/sucrose solutions at temperatures from 293.15 K to 318.15 K," J. Chem. Thermodyn., vol. 133, pp. 123–134, 2019, doi: 10.1016/j.jct.2019.01.024.

# Effect of Temperature and composition on thermophysical properties of Binary liquid mixtures of Propiophenone with Propyl acetate, n-Butyl acetate and n-Pentyl acetate

**S.K.BINDHANI[1]*, Y.K.MOHANTY[2]**

1Department of Chemical Engineering, Gandhi Institute of Engineering and Technology University,
Gunupur 765022, India
[2] Principal, Srinix College of Engineering, Baleswar

In this work, density, viscosity, speed of sound of a binary liquid mixtures of Propiophenone with Propyl acetate, n-Butyl acetate and n-Pentyl acetate have been reported at T= (303.15, 308.15 and 313.15) K and 101.3 kPa. The type of interactions occurring between these two components at different compositions were studied and discussed on the basis of excess molar volume ($V_E$), viscosity deviation ($\Delta\eta$), deviations in speed of sound, acoustical impedance ($\Delta Z$), isentropic compressibility ($\Delta\beta s$), intermolecular free length ($\Delta L_f$), enthalpy ($\Delta H^*$) and entropy change ($\Delta S^*$) calculated from Gibb's energy of activation ($\Delta G^*$). Further a standard response surface methodology (RSM), based on central composite design (CCD) has been used to develop the model equation for predicting the thermodynamic properties.

**References**

[1] T. S. Jyostna and N. Satyanarayana, Indian J. Chem. A 44, (2005).1365
[2] G. S. Manukonda, P. Venkatalakshami, and K. Rambabu, Int. J. Phys. Res. **3** (4), (2013) 5
[3] S. J. Tangeda, S. Boodida, and S. Nallani, J. Chem.Thermodyn. 38, (2006) 1438. [4] A. B. Syeda, R. K. Bachu, A. J. Koppula, S. Boodida,and S. Nallani, J. Chem. Eng. Data 55, (2010) 1067 .
[5] S. L. Oswal, P. Oswal, P. S. Modi, J. P. Dave, R. L. Gardas, Acoust. Thermochim. Acta 1, (2004), 410.
.

# Development of Carbon Dioxide Capture unit for Diesel Engine

**MEHUL KALE, AJIT KUMAR PARWANI*, MAHUYA BANDHYOPADHYAY**

[1]Institute of Infrastructure Technology Research and Management, Ahmedabad 380026, India
*Ajit Kumar Parwani: e-mail: ajitkumar.parwani@iitram.ac.in

**Keywords**: Absorbent, $CO_2$ Capture, pH Values, Electrical Conductivity (EC) Value

Reducing the $CO_2$ emissions of the transportation sector stands out as one of the toughest challenges amidst the energy transition [1]. This research explores the efficiency of various absorbents, including Dimethylethanolamine (DMEA), Monoethanolamine (MEA), Calcium Hydroxide ($Ca(OH)_2$), and Potassium Hydroxide (KOH), in capturing $CO_2$ emissions from a single-cylinder diesel engine's exhaust running at constant speed of 1500 RPM. The absorbents demonstrated successful partial absorption of $CO_2$, leading to reduced emissions. MEA showed the highest $CO_2$ capture efficiency, followed by $Ca(OH)_2$, DMEA, and KOH the $CO_2$ emission on different loads using different absorbents as shown below in Fig.1. However, inconsistencies in emission reductions across different loads and time intervals suggest the influence of additional variables like temperature and pressure. Further studies are required to rectify measurement errors and optimize techniques for carbon capture technology development.

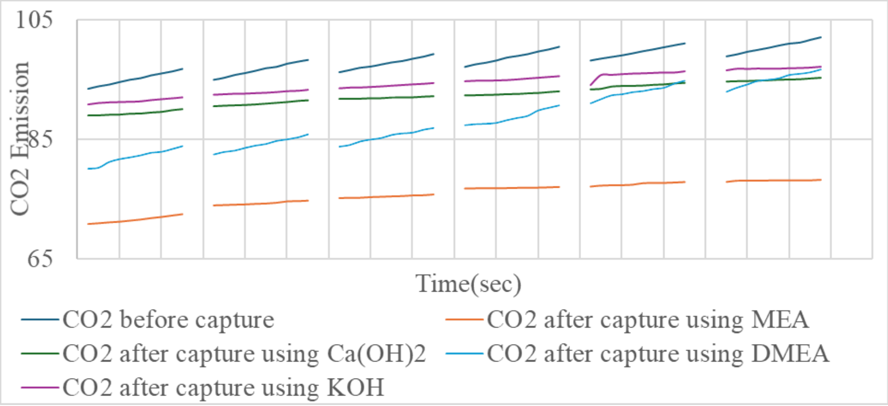


Figure 1:$CO_2$ emission before and after capture using different absorbents

**References**

[1] Kumar, P., Rathod, V., & Parwani, A. K. (2021). Experimental investigation on performance of absorbents for carbon dioxide capture from diesel engine exhaust. Environmental Progress & Sustainable Energy, 40(5), e13651.

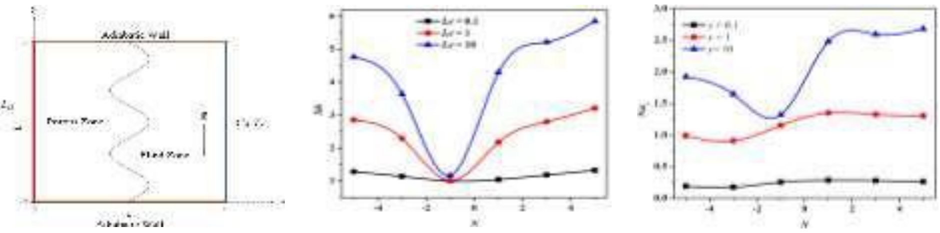
# Double Diffusive Natural Convection within a Partially Saturated Porous Cavity Separated by a Wavy Interface: A Local Thermal Non-Equilibrium Approach

**<u>DEBAYAN BHOWMICK</u>[1]*, DEEPSHIKHA DATTA[2], BIMAL DAS[3]**

[1]Department of Mechanical Engineering, Brainware University, Kolkata – 700125, India
[2] Department of Chemistry, Brainware University, Kolkata – 700125, India
[3]Department of Chemical Engineering, National Institute of Technology Durgapur, Durgapur - 713209, India
*Corresponding author: e-mail: debayanbhowmick2012@gmail.com

**Keywords**: Double diffusive convection; LTNE; Partially porous cavity; Darcy-Brinkman-Forchheiner model.

The present numerical study investigated the influence of porous permeability under local thermal non-equilibrium state within a square cavity partially saturated porous media. The two-dimensional steady flow condition has been maintained along with non-uniform temperature and concentration distribution at the left vertical wall. Moreover, the porous substance has been separated from the free flow region by a wavy interface. To capture the flow physics within the cavity Darcy-Brinkman-Forchhiemer model has been incorporated. The parameters regulating the study are varied as: Darcy number ($10^{-2} \leq Da \leq 10^{-3}$); Rayleigh number ($10^{3} \leq Ra \leq 10^{6}$); Thermal conductivity ratio ($0.01 \leq \gamma \leq 100$); Lewis number ($1 \leq Le \leq 100$) and buoyancy ratio ($-3 \leq N \leq 3$). The outcome of our result indicates that the effect of $Le$ is more significant upon average mass transfer rate ($Sh$) whereas, $\gamma$ and $N$ play dominating role upon the average solid and fluid heat transfer rate. Overall, the impact of LTNE condition is prominent upon the transport phenomena of fluid and thermal. However, it has less impact upon solute distribution.



(a) (b) (c)

Fig. 1: (a) Computational domain (b) Effect of Lewis Number (c) Effect of interphase heat transfer co-efficient

**References**

[1] P. Bera, S. Pippal, A. K. Sharma, *A thermal non-equilibrium approach on double-diffusive natural convection in a square porous-medium cavity*, International Journal of Heat and Mass Transfer, 78 **(2014)** 1080 – 1094.

[2] O. R. Alomar, N. M. Basher, A. A. Yousif, *Natural convection heat transfer from a bank of orthogonal heated plates embedded in a porous medium using LTNE model: A comparison between in-line and staggered arrangements*, International Journal of Thermal Science, **(2021)** 106692.

# Effects of Inclination on Thermal Performance of Closed-Loop Pulsating Heat Pipes

**YOGITA BHATI[1], KAMLESH PARMAR[1,2], AJIT KUMAR PARWANI[1],**
**SUMIT TRIPATHI[1*]**

[1]Department of Mechanical and Aerospace Engineering, Institute of Infrastructure Technology
Research and Management (IITRAM), Ahmedabad-380026, Gujarat, India
[2]Department of Mechanical Engineering, Parul Institute of Engineering and Technology, Vadodara-
391760, Gujarat, India
*sumittripathi@iitram.ac.in

**Keywords:** pulsating heat pipe, thermal resistance, thermal performance

Due to their effective heat transmission qualities, Closed-Loop Pulsating Heat Pipes (CLPHPs) have attained significant interest and are considered viable options for a range of cooling applications in aerospace, electronics, and other industries [1, 2]. This study examines the impact of inclination angle and input heat flow on the thermal performance and operational stability of a CLPHP utilizing deionized water as the working fluid. Specifically, 40% filling ratio (FR) provides optimal thermal resistance at low heat input, and 60% FR provides optimal thermal resistance at high heat input as shown in Fig 1(a). Additionally, it is noted that for high heat input of between 80W and 120W, the thermal resistance achieves its optimal point at 90˚ with the horizontal plane compared to different inclinations as shown in Fig 1(b). The present study provides a comprehensive analysis of different variables affecting thermal resistance in CLPHPs which can be used as a viable thermal management solution with optimum heat transfer rates in various applications.

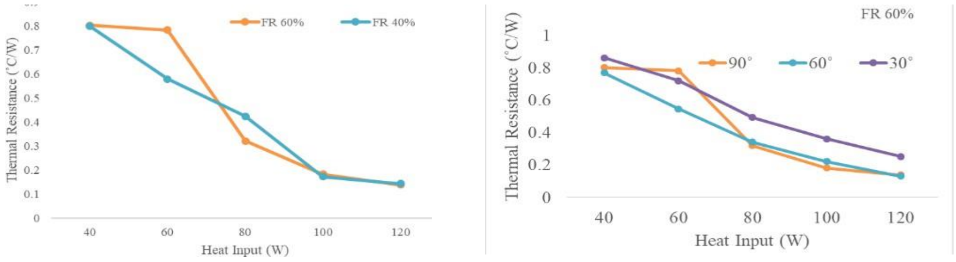


**Fig. 1**: Variation of thermal resistance with heat input (a) at different filling ratio and 90˚ inclination (b) at different inclination and FR 60%

**References**

[1] K. Parmar, I. Nagme, S. Thakur, A. Singh, A. K. Parwani, S. Tripathi, and N. Parmar, Thermal performance comparison of closed loop pulsating heat pipe with DI water and Al2O3/DI nanofluid. *AIP Conference Proceedings,* Vol. 2960, No. 1, AIP Publishing, (**2024**).

[2] M. Mameli, V. Manno, S. Filippeschi, M. Marengo, Thermal instability of a closed loop pulsating heat pipe: combined effect of orientation and filling ratio. *Experimental Thermal and Fluid Science*, 59, (**2014**) 222-229.

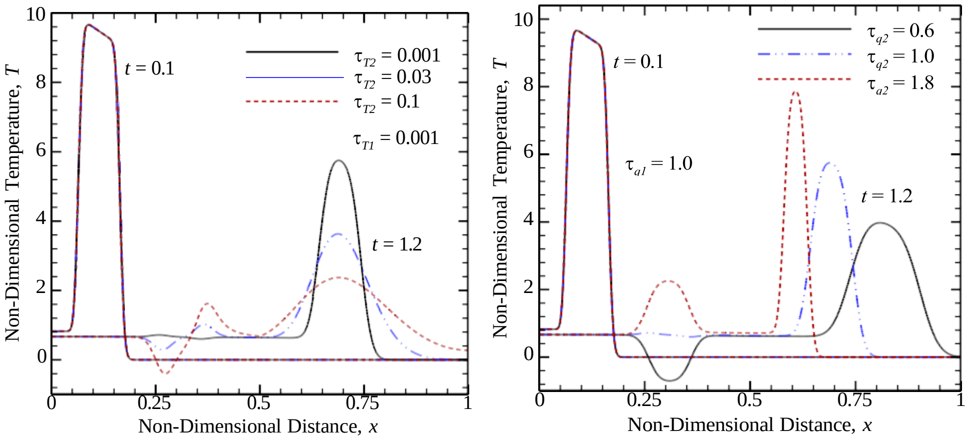
# Interfacial Thermal Characteristics of a Composite Medium Subjected to a Short Pulse Laser Source

**ARNAB LAHIRI**[1]*

[1]Reliability and Quality Assurance Mechanical Systems Group, U.R. Rao Satellite Centre, ISRO, Old Airport Road, Bengaluru-560017
*Corresponding Author: e-mail: a.lahiri2014@gmail.com, arnab@ursc.gov.in

**Keywords**: interface, DPL, temperature, entropy generation

For the last three decades, dual-phase lag (DPL) heat transfer model has found significant applications in solving heat transfer issues arising in non-equilibrium thermal interaction of short-pulse, femtosecond laser pulse with sub-micron spatial domain [1–2]. In this current study, for a given Knudsen number, the role of an ideal & flat interface on thermal energy transport, over small temporal scale is studied.



(a) (b)

Fig. 1 : Spatial variation of temperature over temporal level(s), $t$ = 0.1 & 1.2 for variation of phase-lag of (a) temperature gradient ($\tau_T$) and (b) heat flux ($\tau_q$).

The bi-layered physical domain is subjected to a temporally varying, short pulse laser source at its left boundary. DPL and interfacial heat transport equations are simultaneously solved by an implicit finite difference scheme. The Temporal temperature history and heat flux distributions are depicted and parametric study is conducted to understand the effect of phase lag of heat flux and temperature gradient on thermal energy transport past the interface. Entropy generation characteristics under the frameworks of classical as well as extended irreversible thermodynamics is further studied to assess the thermodynamic consistency of DPL framework.

## References

[1] D. Y. Tzou, *Journal of Heat Transfer* 117 **(1995)** 8.
[2] D. Y. Tzou, *Macro-to Microscale Heat Transfer: The Lagging Behavior.* Taylor & Francis, Washington, DC, 1996.

# Effect of Percentage of Methanol on Micellization Position of Mixed Surfactant Dye Interaction

**CHANDRADIP KUMAR YADAV[1], NEELAM SHAHI[2], TULASI PRASAD NIRAULA[2], AMAR PRASAD YADAV[1], SHOVA NEUPANE[1*], AJAYA BHATTARAI[2*]**

[1]Central Department of Chemistry, Tribhuvan University, Kirtipur, Nepal [2]*Mahendra Morang Adarsh Multiple Campus, Tribhuvan University, Biratnagar, Nepal* Correspondence: bkajaya@yahoo.com or ajaya.bhattarai@mmamc.tu.edu.np (A.B.)

**Keywords**: anionic surfactant, critical micelle concentration, degree of ionization, methyl orange, mixed solvent

The interaction behavior of mixed surfactant-dye systems i.e. anionic surfactant sodium dodecyl sulfate (SDS) and cationic surfactant cetyl pyridinium chloride (CPC) and dye methyl orange (MO) are investigated through the allocation of micelle using conductivity measurements. The critical micelle concentration (CMC) is determined by monitoring the conductivity as a function of surfactant concentration. The results showed a sharp increase in the conductivity with increasing surfactant concentration. Also, the conductivity of electrolytes increases with an increase in temperature whereas the conductivity of electrolytes decreases with an increase in the amount of methanol. Methanol-water mixed dissolvable media containing 0.00, 0.10, 0.20, and 0.30 volume parts of methanol at 298.15, 308.15, and 318.15 K to work out the basic micelle fixation, gives significant understanding to the arrangement conduct of the mixed surfactants. The CMC and degree of micellar dissociation (α) of SDS in the presence of CPC increase in the methanol–water, mixed solvent medium. The CMC value is increased on increasing the temperature. The micellization's thermodynamic functions are computed under various circumstances. Because of the creation of a molecular complex in mixed surfactant systems, micellization becomes more probable with MO. Various thermodynamic parameters (ΔGo, ΔHo, ΔSo), were computed in mixed surfactant in the presence of MO.

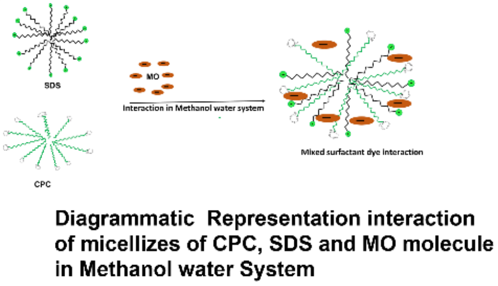


Fig. 1: Mixed Surfactant dye interaction

**References**

[1] K.M. Sachin, S. Karpe, M. Singh, A. Bhattarai, *Macromol. Symp.*, 379 (**2018**).
[2] N. Shahi, S. Kumar Shah, A. Prasad Yadav, A. Bhattarai, *Results Chem.*, 5 (**2023**) 100906.

# NUMERICAL STUDY ON HEAT DISTRIBUTION AND EFFECT OF BURNER CONFIGURATION IN PLATE CONVEYORS

**NOEL REBU SAM[1], ADARSH.R[1], BIJAY.N.J[1], HARISANKAR.R[1], K.E. REBY ROY[2]***

[1] Research Scholar, Dept. of Mech. Engg., TKM College of Engineering, Kollam-691005, India
[2] Professor, Dept. of Mech. Engg., TKM College of Engineering, Kollam-691005, India
*Corresponding author: e-mail: rebyroy@tkmce.ac.in

**Keywords:** Uniform heat distribution, burner configurations, standard deviation

Achieving uniform heat distribution in a plate conveyor is crucial for efficient operation, reducing energy consumption, and improving product quality in industrial applications. Studies have shown the advantages of using conveyor belt systems for baking processes, such as catalytic infrared radiation for dried tofu baking [1]. The present study examines the heat distribution uniformity on a Plate conveyor system featuring four burner configurations: parallel, parallel with adjusted spacing, zigzag, and slanting. The influence of plate motion on heat distribution uniformity is assessed by comparing results between stationary and moving plate configurations.

We employed ANSYS Fluent software to simulate heat transfer processes using mesh and solid motion techniques. The four-burner configurations were analyzed under both steady and transient conditions. Heat distribution uniformity was quantified using the standard deviation of temperature distribution from the mean temperature across the plate surface. Heat transfer efficiency was assessed through heat transfer coefficients and Nusselt numbers. Temperature profiles along the plate's axes were plotted to visually evaluate the uniformity of heat distribution across different burner configurations and motion states. In addition, our methodology was validated by comparing simulation results with experimental data from Corlay and Advani [2].

Our analysis demonstrated that the 'Parallel with adjusted spacing' configuration provided the best uniform heat distribution for a stationary plate conveyor, with a standard deviation of temperature from the mean value to be 4.934 K. For moving plate conveyors, the 'Slanting configuration' was the most effective, with a standard deviation of 6.3191 K. This approach can be applied in industries that require precise and consistent heating processes, thereby enhancing overall thermal efficiency.

**References**

[1] Wenqing Chen, Chen Shen, Qunhui Jiang, Conveyor belt catalytic infrared radiation as a novel apparatus for dried tofu baking: Focus on evaluation of physicochemical qualities, Innovative Food Science and Emerging Technologies, 2024

[2] C. Corlay, S.G. Advani, Temperature distribution in a thin composite plate exposed to a concentrated heat source, Internation Journal of Heat and Mass Transfer, 2007

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

---

## Abstract for ICTAC 2024

# Thermodynamic Studies of Energetics of Ionic Interactions for Aqueous Choline Carboxylate Bio-ionic liquids at 298.15 K.

Pratiksha P, Gavhane[1], Deepti N. Kurhe[2], Guruprasad J. Hasolkar[1] and Dilip H. Dagade[1*]
[1]*Department of Chemistry, Shivaji University, Kolhapur – 416 004*
[2]*Department of Biotechnology, Shivaji University, Kolhapur – 416 004*
*Corresponding author: e-mail: dhd_chem@unishivaji.ac.in

**Keywords**: osmotic coefficient, bio-ionic liquids, molecular interactions, etc.

Bio-ionic liquids are one of those important findings of researchers as being totally composed of bioderived ionic alterations, and hence provided opportunities for their applications in many different areas like electrochemistry, pharmaceutics, etc. Since last two decades, choline-based ionic liquids have selectively emerged to be versatile due to their non-toxic, biodegradable nature. In present work, choline carboxylate ionic liquids comprised with Choline [CHOL] as a common cation with various anions viz. Lactate [LAC], Pyruvate [PYR], Glucuronate [GLN] and Galacturonate [GLC] have been synthesized and their osmotic coefficients were measured over concentration range of ~0.02 to ~1.00 mol·kg$^{-1}$ at 298.15K. From the experimental data of osmotic coefficient, water activity, mean molal activity coefficients of bio-ILs were determined to estimate mixing and excess Gibbs free energy changes. The non-electrolyte contribution to the aqueous solutions of studied bio-ILs were evaluated through application of McMillan-Mayer theory of solutions from activity coefficients in terms of osmotic second virial coefficient which signifies electrically neutral ion-pair – ion-pair interactions in aqueous bio-IL solutions. Osmotic coefficient data was again scrutinized to determine significant Pitzer ion interactions parameters ($\beta^{(0)}$) and ($\beta^{(1)}$) by using a nonlinear least-square fit method for fitting osmotic coefficient data using Pitzer madel for 1:1 electrolytes. The osmotic second virial coefficients found to be positive for all the studied ILs signify the presence of repulsive type of ion-pair–ion-pair interactions. Whereas the negative values obtained for ($\beta^{(1)}$) of [CHOL][LAC] and [CHOL][PYR] and positive values in case of [CHOL][GLN] and [CHOL][GLC] which indicates the oppositely charge ion interactions and like charge ion interactions in water respectively. The results have been further interpreted in terms of ionic hydration, ion-ion interactions, cooperative H-bonding, water structural changes, etc.

**References:**

1. B. L. Gadilohar, G. S. Shankarling, *J. Mol. Liq.* 227 (**2017**) 234-261.
2. S. P. Shinde, and D. H. Dagade, *J. Chem. Eng. Data*, 60, (**2015**) 635–642.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Designing and developing an intelligent control system to be applicable for different heating and cooling applications

**DAMANBHA MARWEIN, PIYUSH YADAV, OMPRAKASH YADAV, BIPLAB K. DEBNATH*, RAJAT S. DAS**

National Institute of Technology Meghalaya, Shillong, Meghalaya-793003, India
* Corresponding author: biplab.debnath@nitm.ac.in

**Keywords**: Heating, cooling, control system, heating element, cooling fan.

Heating and cooling play crucial roles in various thermal applications, ensuring comfort, safety and efficiency. With technological advancements, there has been a significant shift towards automatic control of these parameters, optimizing performance and energy consumption. This present study aims to develop and design an intelligent control system for heating and cooling purposes. In the heating aspect, a control system is implemented using a real-time clock (RTC) module to allow users to set specific times for heating operations. Additionally, a switch sensor equipped with an environmental illumination automatic detection circuit is employed to control the heating process, automatically shutting down during the day and activating at night. This information is managed by a programmed code that directs the heaters to turn on automatically and determines their duty cycle. The heaters used in this experimental study utilizes a PTC thermistor as the heating element and have a surface dry heating temperature of 220°C. Water is used as the heating medium, with different duty cycles set to maintain the desired temperatures. For the cooling part, five small 12V fans are integrated with the circuit, adjusting their speed based on temperature readings from the code. The DS18B20 temperature sensor is utilized to monitor the water temperature, which varies from 15°C to 50°C. Different duty cycles were set into the code for various temperature ranges. At a 100% duty cycle, the individual fan achieved an output of 2569 rpm, generating an air velocity of 1.45 m/s and a flow rate of 0.0089 kg/s. Here, 100% duty cycle works at a temperature of 50°C and above. Accordingly, below 50°C and above 15°C three more equispaced duty cycles (75%, 50% and 25%) are considered. The ranges in the duty cycles can also be adjusted based on the application in which it may be applied. The control system is designed to work at these ranges, automatically and effectively. This paper outlines the study and highlights the necessity of automated heating and cooling systems in various thermal applications, namely, air-conditioning and refrigeration, solar air heater, solar still, etc. emphasizing their efficiency and potential to enhance energy management.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Effect of Zinc Additive on Thermal Transport Properties of Novel Multicomponent Chalcogenide Se-Te-Sn System: Transient Plane Source Technique

**DEEPAK KUMAR[1], KRISHNA PAL[1], ARVIND KUMAR SHARMAB[2], HORESH KUMAR[3], KEDAR SINGH[4], SUNIL KUMARA[1]****

[1]Department of Physics, Government Post Graduate College, Bisalpur, Pilibhit, 262201 U.P. India
[2]Department of Physics, School of Physical Science, Mahatma Gandhi Central University, Motihari-845401, Bihar
[3]Department of Physics, Institute of Science, Banaras Hindu University, Varanasi,221005, U.P. India
[4]School of Physical Science, Jawaharlal Nehru University, New Delhi, 110067 India
*Corresponding author: e-mail: l: skcbhu07@gmail.com

**Keywords**: Multi-Component Chalcogenide, Transient Plane Source Technique Thermal Conductivity, Thermal Diffusivity, Specific Heat Per Unit Volume, Constraint Theory

This research delves into the thermal transport characteristics of the novel multi-component chalcogenide Se90-xTe5Sn5Znx (0≤x≤9) (STSZ) system, which was prepared using the melt quenching method. The thermal conductivity, thermal diffusivity, and specific heat per unit volume of twin pellets of STSZ chalcogenide glasses were measured at room temperature by using a transient plane source (TPS) technique. The findings revealed that the thermal transport properties, including thermal conductivity, thermal diffusivity, and specific heat per unit volume, revealed an optimal change corresponding to 6 at. % of Zn in the STSZ matrix. This variation in thermal transport properties based on composition can be accredited to the structural relaxation behavior of the multi-component quaternary matrix of STSZ. Additionally, the observed variations in the thermal transport properties of the STSZ matrix can be clarified using a topological model based on constraint theory.

# Thermodynamic model for pressure evolution during in-flight active pressurisation of liquid hydrogen tank of a cryogenic upper stage

**Avinash Kumar Yadav[1]*, Deepak V M[1], Paramasivam P[1]**

[1]Liquid Propulsion Systems Centre, Indian Space Research Organisation,
Thiruvananthapuram-695547, India
*Corresponding author: avi.yadav111993@gmail.com

**Keywords**: thermal analysis, active pressurisation, LH2 tank, evaporation

Active pressurisation of a cryogenic liquid hydrogen (LH2) tank is carried out using non-condensable gaseous helium (GHe). A thermodynamic model, incorporating the heat transfer aspects for the gas bottle, pressurisation line and tank ullage, is developed to predict the pressurisation rate during the in-flight active pressurisation of LH2 tank. The predicted value of pressurisation rate is found to be 13% lower than the achieved pressurisation rate due to under-estimation of evaporation rate. Accordingly, the model is updated by modifying the correlations used for estimating the mass transfer across the liquid-vapor interface. The updated model results are validated with the flight data and is used to predict the pressurisation rate for the next flight. The difference in pressurisation rate is found to have reduced to 2% by including the effect of evaporation on tank pressure evolution. Therefore, accurate estimation of evaporation rate plays a crucial role in predicting the rate of pressurisation of LH2 tank.

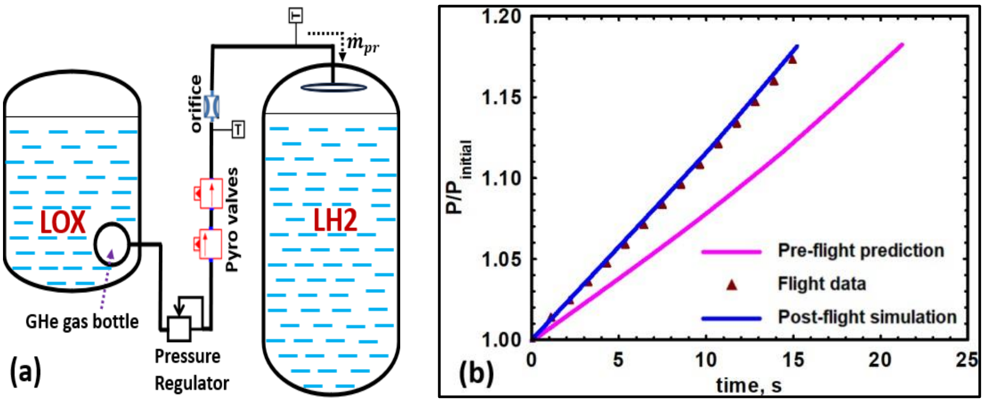


Fig. 1 :(a) Schematic of active pressurisation circuit (b) Model results

**References**

[1] A Ludwig C, Dreyer ME. Investigations on thermodynamic phenomena of the active pressurization process of a cryogenic propellant tank. Cryogenics (2014), 63:1

[2] J. H. Corpening, Analytic modeling of pressurization and cryogenic propellant conditions propellant conditions for lunar landing vehicle. *57th JANNAF joint propulsion meeting*, May 2010, Colorado Springs, CO

[3] Z. Zou, A review of cryogenic quasi-steady liquid-vapor phase change: Theories, models, and state-of-the-art applications, International Journal of Heat and Mass Transfer, (2023), 205, 123916

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Exploring properties of Protein Fibrils from Self-Assembly to Drug Delivery: Thermodynamic analysis

**ANU JAIN*, NAND KISHORE**

Department of Chemistry, Indian Institute of Technology Bombay, Mumbai 400076, India
*Corresponding author: e-mail: nandk@iitb.ac.in

**Keywords**: Isothermal titration calorimetry; Differential scanning calorimetry; Spectroscopy; Protein fibrillation; Pluronic

Understanding misfolding and aggregation of proteins is important in disciplines of proteins, pharmaceutical, and biomedical fields. Protein misfolding and assembly results in formation of amyloid fibrils leading to crippling conditions referred to as "amyloidosis” [1,2]. They are fundamentally robust and insoluble nanofibers with considerable potential as nanotechnology and bionanotechnology materials. This work examines lysozyme fibrillation in the presence of pluronics (F68 and F127) using combination of calorimetry and spectroscopy. Pluronic copolymers self-assemble to form polymeric micelles, or micellar-type nanostructures in aqueous solution, at concentrations higher than critical micellar concentration. The results obtained from isothermal titration calorimetry suggest that interaction of protein with F68 is exothermic while with F127 it is endothermic due to more hydrophobicity of the latter pluronic. TEM images and ThT assay demonstrated that pluronics promoted fibrillation process rather than inhibiting it. The pre- and post-micellar concentrations of pluronics on interaction with protein (at varying fibrillation stages) exhibit a reduction in $\Delta H_m^0$ value as the incubation time increases. Consequently, the potential use of these formed aggregates for drug delivery was explored using two anticancer drugs (5-fluorouracil and cytarabine). When cytarabine is used with protein fibrils, the hydrophobic interaction predominates, according to endothermic enthalpy of interaction, but the electrostatic interaction predominates with 5-flourouracil. On the other hand, the former drug exhibited more adsorption on the surface of protein fibrils compared to the latter. Therefore, it is concluded that cytarabine has weak adsorption on fibril surfaces and is readily desorbed in cells, whereas 5-fluorouracil has relatively strong adsorption; as a result, the complex of LFF127 and 5-FU is fatal to malignant cells. These results are beneficial for exploring numerous applications of the formed protein fibrils/aggregates and in providing suitable strategies for the design and development of drug delivery agents.

**References**

[1] P. Ghosh, P. De, ACS Appl Bio Mater 3 (2020) 6598–6625.

[2] J.D. Sipe, M.D. Benson, J.N. Buxbaum, S. Ikeda, G. Merlini, M.J.M. Saraiva, P. Westermark, Amyloid 23 (2016) 209–213.

**T1- OP 23**

# Investigation of molecular interaction between 1-butyl-3-methyl-imidazolium hexafluorophosphate with Propyl acetate

T. S. Krishna[1]*****, K. Narendra[2]

[1]Department of Physics, P B Siddhartha College of Arts & Science, Vijayawada-520010, India
[2] Department of Physics, V R Siddhartha School of Engineering, SAHE, Vijayawada-520007, India
*Corresponding author: sritadikonda@gmail.com

**Keywords**: Density; speed of sound; Propyl acetate; Ionic Liquids; intermolecular interaction

The speeds of sound, *u* and densities, □, of the blends, of various Imidazolium based Ionic liquids with Propyl acetate including those of pure liquids, have been determined from 0 to 0.1 mole fraction range of ILs with interval 0.1 at 298.15 - 323.15 K at pressure 0.1MPa. We used the measured data to assess the excess molar volumes, $V_m^E$, excess isentropic compressibility, $\square_s^E$, excess speeds of sound, $u^E$, excess molar isentropic compressibility, $K_{s,m}^E$, excess isobaric thermal expansion, $\alpha_p^E$, were calculated and fitted with the Redlich-Kister equation. The excess partial molar volumes, $\bar{V}_{m,1}^E$ and $\bar{V}_{m,2}^E$ and excess partial molar isentropic compressibilities, $\bar{K}_{s,m,1}^E$ and $\bar{K}_{s,m,2}^E$, excess partial molar volumes, $\bar{V}_{m,1}^{\circ E}$ and $\bar{V}_{m,2}^{\circ E}$ and excess partial molar isentropic compressibilities, $\bar{K}_{s,m,1}^{\square E}$ and $\bar{K}_{s,m,2}^{\circ E}$ of the components at infinite dilution have also been measured. The departure of measured properties has been explored in terms of intermolecular interactions.

**References**
[1] Mohammed Taghi Zafarani-Moattar, Hemayat Shekaari. J. Chem. Thermodyn., 38 (2006) 1377–1384.
[2] J. Pandurangarao, K. Narendra, V. Vishalakshma, T. S. Krishna, G. Srinivasa Rao, J. Chem. Thermodyn., 190(2024) 107222.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Unlocking Efficiency: A Comprehensive Review of Advanced Techniques for Optimizing Solar Air Heater

**BRAJESH KUMAR AHIRWAR[1]*, ARVIND KUMAR[2]**
[1,2]Department of Mechanical Engineering, Maulana Azad National Institute of Technology, Bhopal
Madhya Pradesh 462003, India
*Corresponding author: e-mail: 203116025@stu.manit.ac.in

**Keywords**: Solar air heater, Turbulators, Protrusion, Efficiency, Artificial roughness

**Abstract:**

Energy is the fundamental force that drives life. It is essential for the growth, advancement, modernization, and economic development of any nation. To meet the rising energy demand and protect the planet from pollution, the global focus is shifting from fossil fuels to renewable energy sources. Among these emerging energy sources, solar power is becoming increasingly important. Solar air heaters are crucial for capturing solar energy, but their efficiency is hindered by low thermal performance. This inefficiency is primarily caused by the formation of a laminar sub-layer on the absorbing plate. This review article outlines various techniques for improving the efficiency of solar air heaters (SAHs) by disrupting the laminar sub-layer. It focuses on methods such as artificial roughness, jet impingement, and piezoelectric fans, all employed to enhance the performance of SAHs. This article also discusses the use of phase change materials (PCMs) to improve the performance and efficiency of SAHs. This review aims to update readers on recent advancements, challenges, and future prospects of solar air heaters (SAHs) as an alternative to fossil fuels. It concludes by evaluating the advantages and disadvantages of SAHs and offers recommendations for future research to expedite their commercial adoption.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# THERMAL PERFORMANCE ANALYSIS OF AN OVAL DOUBLE-PIPE HEAT EXCHANGER IN A POROUS MEDIUM USING FINITE VOLUME METHOD

**GIZELLE RODRIGUES[1], NEETU SRIVASTAVA[2]***

[1, 2] Department of Mathematics, Amrita School of Engineering, Amrita Vishwa Vidyapeetham,
Bengaluru – 560035, India
*Corresponding author: email: s_neetu@blr.amrita.edu

**Keywords**: Oval Double Pipe Heat Exchanger, Finite Volume Method, Heat Transfer, Porous Medium

In this paper, we conduct an axisymmetrical numerical investigation to improve the heat exchange performance of an oval double pipe heat exchanger (DPHE) filled with a porous medium. The Darcy-Brinkman-Forchheimer model is utilized to describe the steady flow within the porous region, and the Finite Volume Method is employed to solve the governing equations with suitable boundary conditions. The results highlight the importance of porous media in enhancing the performance of an oval DPHE under steady flow conditions, demonstrating significant improvements in heat exchange efficiency.

**References**

[1] Chen, W. L., & Dung, W. C. (2008). Numerical study on heat transfer characteristics of double tube heat exchangers with alternating horizontal or vertical oval cross section pipes as inner tubes. *Energy Conversion and Management*, *49*(6), 1574-1583.

[2] Shirvan, K. M., Mirzakhanlari, S., Kalogirou, S. A., Öztop, H. F., & Mamourian, M. (2017). Heat transfer and sensitivity analysis in a double pipe heat exchanger filled with porous medium. *International Journal of Thermal Sciences*, *121*, 124-137.

[3] Luo, C., Song, K., & Tagawa, T. (2021). Heat transfer enhancement of a double pipe heat exchanger by Co-Twisting oval pipes with unequal twist pitches. *Case Studies in Thermal Engineering*, *28*, 101411.

# Enhanced Micellization and Structural Transformation in Morpholinium-Based Ionic Liquids with Aromatic Counterions

**SANJAY H. PANJABI[1]*, RAVI VIRADIYA[1], V K ASWAL[2]**

[1]Chemical Sciences Department, P D Patel Institute of Applied Sciences, Charotar University of Science and Technology, Changa, Gujarat, India -388421
[2]Solid State Physics Division, Bhabha Atomic Research Center (BARC), Mumbai 400085, India;

**Keywords**: Surface-active ionic liquids, Aromatic counterions, Micellization, Small-angle neutron scattering

In this study, we synthesized two novel morpholinium-based surface-active ionic liquids (SAILs) with aromatic counterions: n-dodecyl-n-methylmorpholinium salicylate ([$C_{12}$mmor][Sal]) and n-dodecyl-n-methylmorpholinium 3-hydroxy-2-naphthoate ([$C_{12}$mmor][3-H-2-n]). We systematically explored their aggregation behavior in aqueous solutions using various analytical techniques, including electrical conductivity, small-angle neutron scattering (SANS), surface tension measurements, and UV-Vis spectroscopy. Our findings revealed that incorporating aromatic counterions enhances the micellization properties compared to conventional halogenated SAILs such as [$C_{12}$mmor][Br]. SANS analysis showed a structural transformation from prolate ellipsoidal micelles to large unilamellar vesicles when the counterion was changed from salicylate to 3-hydroxy-2-naphthoate. Thermogravimetric analysis (TGA) was employed to assess the thermal stability of the synthesized SAILs. The TGA results indicated high thermal stability for both [C12mmor][Sal] and [C12mmor][3-h-2-n], which is crucial for their potential applications in various high-temperature processes. Additionally, we observed that increasing the concentration of [$C_{12}$mmor][Sal] resulted in a lower aggregation number. We present comprehensive thermodynamic, micellar, and interfacial parameters, including the degree of counterion binding (β), critical micelle concentration (CMC), minimum area per molecule ($A_{min}$), surface excess concentration ($\Gamma_{max}$), standard Gibbs free energy of adsorption ($\Delta G_{ad}°$), aggregation number (Nagg), standard Gibbs free energy of micellization ($\Delta G_{m}°$), standard enthalpy of micelle formation ($\Delta H_{m}°$), and standard entropy of micellization ($\Delta S_{m}°$). This study underscores the potential of aromatic counterions in morpholinium-based SAILs to improve micellization properties, offering new insights into the design of efficient and environmentally friendly surfactants. The results have significant implications for various applications, including catalysis, drug delivery, and materials science.

# DECIPHERING THE BINDING INTERACTIONS OF ANTI-CANCER DRUGS USING MULTI-SPECTROSCOPIC TECHNIQUES AND *IN-SILICO* METHODS

**INSHA AKBAR [1], SAMIMA KHATUN[2], ADIL MAHAMMAD[3], RIYAZUDDEEN[1]***

1,2,3 University Department of Chemistry, Aligarh Muslim University, Aligarh 202002, India
*rz1@rediffmail.com

**Keywords**: Procarbazine, Pixantrone, spectroscopic techniques, Stern-Volmer analysis.

The binding interaction studies of two different classes of oncotherapeutic drugs, Alkylating agent and Anthracenedione, *viz*., Procarbazine (PCZ) and Pixantrone (PXN) respectively with Hen egg white Lysozyme (HEWL) was investigated employing multi-spectroscopic techniques and *in-silico* studies. Stern-Volmer analysis of fluorescence evidenced that both the anti-cancer drugs quench the intrinsic fluorescence spectra of lysozyme via static quenching mechanism. PCZ demonstrated comparatively stronger binding affinity towards lysozyme with binding constants, K $10^4$ and $10^3$ for PCZ and PXN respectively at T = 298.15 K. The two drugs were found to led to increment in the polarity around Trp amino acid units as evidenced by synchronous and 3D spectral studies. Binding of the drugs resulted in significant alterations in secondary structure of lysozyme was confirmed by CD and FT-IR studies. Furthermore, computational studies provided the atomistic information related to binding of both the drugs and further validated the higher binding of PCZ over PXN. DFT and SIMULATION studies provided deep insights of binding of drugs in accordance with the experimental observations and results obtained.

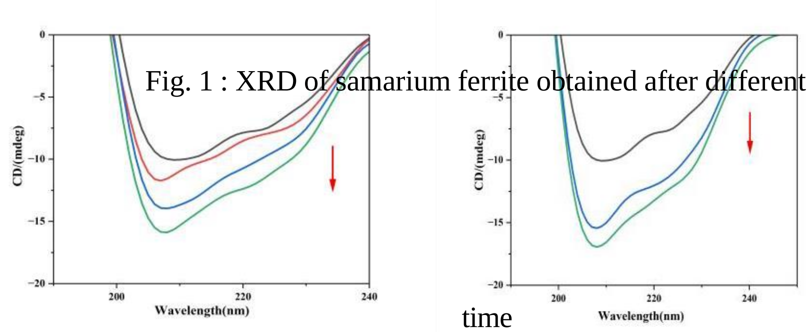


Fig. 1 : XRD of samarium ferrite obtained after different a time

Fig.1: Far-UV CD spectra of HEWL in in absence and presence of (a) PXN (b) PCZ at T =298.15 K and pH 7.4

## References

[1] Iraz Çinar, İrem Aksoy, Günnur Güler*, Turkey, **(2020)** “978-1-7281-8073-1/20/$31.00 ©2020 IEEE”

[2] Sood, D., Kumar, N., Rathee, G., Singh, A., Tomar, V., &amp; Chandra,R. Scientific Reports, Delhi, **(2018),** 8(1).

[3] Saha, S., &amp; Chowdhury, J. Journal of Photochemistry and Photobiology B: Biology, Kolkata,193, **(2019),** 89-99.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

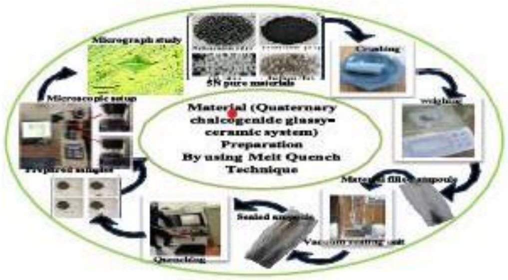
# Studying the Mayer-Neldel rule and crystallization kinetics in STSI glassy systems using iso-conversional approaches

**KAUSHAL K. SARSWAT[1], NEERAJ MEHTA[1*]**

[1]Material Science Lab, Dept of Physics, Banaras Hindu University,
*Corresponding author: e-mail: dr_neeraj_mehta@yahoo.co.in & kksaraswat@bhu.ac.in

**Keywords**: thermal analysis, DSC, MN Rule, isoconversional

This study explores the glass-to-crystal phase transformation in a newly developed chalcogenide glass system, Se-Te-Sn-In (STSI). Researchers synthesized a range of STSI glasses with different indium (In) concentrations (Se78-xTe20Sn2Inx, where x = 0, 2, 4, and 6) and performed comprehensive thermal, structural, and thermomechanical analyses. The study utilized Differential Scanning Calorimetry Characterizing Thermal and Mechanical Properties in Indium-Doped Metal Chalcogenide Glasses (DSC) to analyse the thermal behaviour of the glass, revealing a significant increase in the crystallization rate with the addition of indium to the base Se-Te-Sn glass. As indium content increased, the average heat of atomization and overall mean bond energy decreased, indicating a reduction in the cohesive energy of the samples. An inverse relationship was found between the thermal stability parameter and the enthalpy released during the glass-to-crystalline phase transformation. (Material Synthesis Process) Micro-indentation tests were conducted to assess mechanical properties, including hardness, modulus of elasticity, minimal micro-void formation energy, glass fragility index, and micro-void volume. The covalent nature of the glassy system was examined, and findings on fracture toughness and crack patterns were reported. This study offers valuable insights into the glass-to-crystal phase transformation and the associated physicochemical properties of the innovative STSI chalcogenide glass system. These findings have potential implications for various technological applications.



**References**

[1] Bong Je. Park, Electrochemical Society Meeting Abstracts 229. No. 24. *The Electrochemical Society, Inc*., 2016.
[2] N. Chandel, N. Mehta, *Journal of Physics and Chemistry of Solids*, 115 (**2018**), 113-118

**T1- OP 29**

# Analysing the thermohydraulic performance of a double pass solar air heater integrated with triangular grooves

**KRITTIKA PATWARI[1]*, RAJAT SUBHRA DAS[2]**

[1,2] National Institute of Technology Meghalaya *Corresponding
author: e-mail: p22me017@nitm.ac.in

**Keywords**: DPSAH, triangular grooves, THPP, blockage ratio

The heat transfer enhancement in a double pass solar air heater (DPSAH), while keeping the pressure losses minimum, is investigated numerically in this work. An imposition of a constant heat flux of 880W/m$^2$ is considered to mimic realistic solar irradiation condition. The uniqueness of the design of the DPSAH, which contributed to its superior performance, lies in the formation of triangular grooves attached on the lower side of the absorber plate. Twenty-five simulations on the 3D modelling of computational domain is carried out by using commercially available Ansys Fluent 23.0 software. The RNG k-ε turbulence model with enhanced wall treatment has been used to solve the governing equations. The length, breadth and height of the DPSAH are taken to be 1014mm, 350mm and 72mm respectively. Prime investigation is to observe the impact of triangular grooves on Nusselt number (*Nu*) and friction factor (*f*) by varying the blockage ratio *(e/H)* with Reynolds number *(Re)*. The considered range of *e/H* and *Re* is 0.4-0.8 and 3000-11000 respectively. By changing *e/H* for different values of *Re* the performance of the DPSAH is analysed by considering the factors such as Nusselt number *(Nu)*, friction factor *(f)*, thermal enhancement factor ($Nu_{tri}/Nu_{flat}$) and friction enhancement factor ($f_{tri}/f_{flat}$). A maximum THPP of 3.96 has been obtained at *e/H* of 0.7 when *Re* is maintained at 11,000, which indicates the remarkable improvement in thermo-hydraulic performance of the triangular grooved DPSAH compared to a flat-plated counterpart, by positively impacting the thermo-fluid characteristics within the domain of the heat-exchanging conduit.

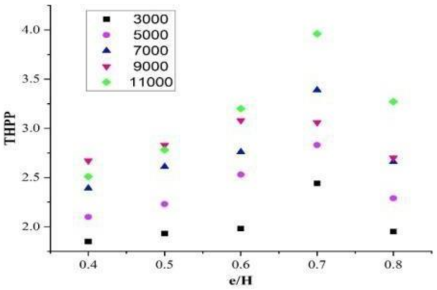


**Fig. 1** Variation in THPP with e/H for different values of Re

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermal management analysis of electric vehicles using low GWP refrigerants

**Md Jamil Akhtar*[1], S.P.S. Rajput[2]**

[1,2]Department of Mechanical Engineering, M.A.N.I.T., Bhopal, India
Corresponding Author: jamil8492@gmail.com

**Keywords:** thermal management, EVs, R1234ze, R134a, refrigerant direct cooling

The thermal management (TM) system of electric vehicles (EVs) lithium-ion batteries based is of great importance because it effects the performance, longevity, and efficiency of the system. A refrigerant direct cooling (DC) have been gradually developed due to high battery energy density. Refrigerant R134a, is frequently utilized in TM of EVs, may be gradually curtailed due to its high Global Warming Potential (GWP). A small-scale experimental installation is built in this study to test a dual refrigeration loop system that can be used for battery DC and AC in electric vehicle cabins. In two cooling modes of the R134a system, the refrigeration performance of R1234ze as direct replacements for R134a is tested, and the effect of refrigerant amount (RA) on system cooling performance is discussed for low-GWP refrigerants at different ExV openings maintaining the same compressor speed. According to the results, for both cooling modes, the ideal RA for R134a, R1234ze are 700g, 650g respectively. Although R134a can be readily replaced by R1234ze in current systems, each has unique benefits and drawbacks. The discharge temperature (DT) at R1234ze is the lowest. R1234ze displays a 21.11% and 19.26% fall in coefficient of performance (COP) over R134a.

## References

[1] A. Khan, *J. Energy Storage*, vol. 76(**2023**), 109852.
[2] F. S. Hwang, *Energy Rev.*, 192(**2022**), 114171.
[3] X. Zhang, Q. Gao, S. Yang, Y. Gao, and T. Zhang, *Appl. Therm. Eng.*, 226(**2023**), 120306.
[4] S. Kharabati and S. Saedodin, *J. Energy Storage*, 75(**2023**), 109586.

T1- OP 31

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

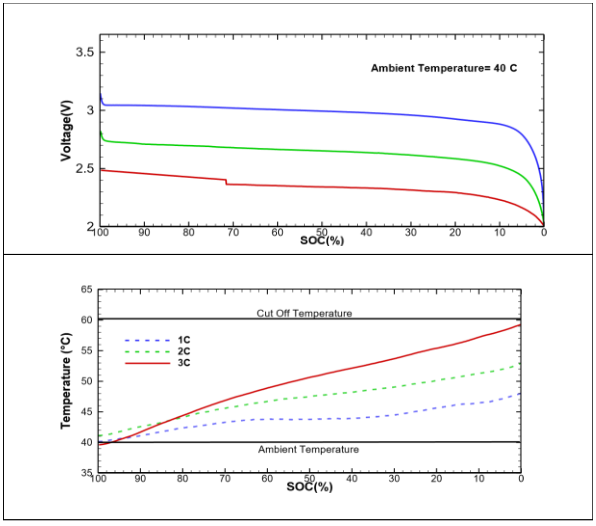
# Electro-Thermal Analysis of single LFP Cell

**MIHIR PANDYA[1]*, DR. HEMANTKUMAR B. MEHTA[1], DR. VIPUL M. PATEL[1]**

[1] Department of Mechanical Engineering, SVNIT Surat, Gujarat, 395007, India *Corresponding author: e-mail: d20me015@med.svnit.ac.in

**Keywords**: LFP cell, Heat generation analysis, Battery thermal management, Thermal Runway.

An experimental analysis of the electro-thermal behaviour of a 32700 LFP (lithium ferro-phosphate) cell with a capacity of 3.2V and 6Ah under different ambient temperature condition (20°C, 30°C, and 40°C) conducted. The cell was tested at various C-rates (1C, 2C and 3C rates) during discharging. Temperatures at the positive node, center, and negative node were measured for each rate. At an ambient temperature of 30 °C, the battery produces average heat outputs of 2.75808 W at 1C discharge rate, 5.1616 W at 2C discharge rate, and 6.9835 W at 3C discharge rate, with full discharge. At an ambient temperature of 40 °C, the battery generates average heat outputs of 3.01 W at 1C discharge rate, 5.048 W at 2C discharge rate, and 6.81 W at 3C discharge rate, with full discharge. The results indicate that as Crates increase ( from 1C to 3C rate), the cell temperature rises. Additionally, higher C-rates and increased ambient temperature( from 20°C to 40°C ) elevate the risk of thermal runaway.



## References:

[1] K. Yang, J. J. An & S. Chen, *Journal of Thermal Analysis and Calorimetry*, *99*(2) (**2009**) 515–521.

[2] K. Fang, S.Chen, D.Mu, J. Liu, & W. Zhang, *Journal of Thermal Analysis and Calorimetry*, *112*(2) (**2012**) 977–981.

[3] Z.W Zhao, G.Y Zhang, L.Yang, J.X. Qiang, & Z. Q.Chen, *Journal of Thermal Analysis and Calorimetry*, *104*(2) (**2010**) 561–567.

[4] M. Vachhani, K. R. Sagar, Patel, M. Vipul, & H.B. Mehta, *Journal of Thermal Analysis and Calorimetry*, *148*(23) (**2023**) 13639–13654.

[5] M. Vachhani, K.R. Sagar, D.N. Jha, Patel, Vipul. M., & Mehta, H. B, *Energy Sources, Part A: Recovery, Utilization, and Environmental Effects*, *46*(1) (**2023**) 689–705.

**T1- OP 32**

# Thermophysical Properties, FT-IR and Computational studies on molecular interactions of Chlorobenzene with isomeric cresols

**N. Hari Krishna[1], Sreenivasulu Karlapudi[2], S. Ravi Kumar[3], R. Karthik[3], Kasibhatta Siva Kumar[4], P. Venkateswarlu[1*]**

[1]Department of Chemistry, Annamacharya Institute of Technology and Sciences, Tirupati-517507, Andhra Pradesh, India.
[2]Department of Chemistry, Sree Rama Engineering College, Tirupati-517507, Andhra Pradesh, India.
[3]Department of Physics, Saveetha School of Engineering, SIMATS University, Tamilnadu- 602105, India.
[4]Department of Chemistry, S.V. Arts college (T.T.D'S), Tirupati-517502, Andhra Pradesh, India.
*Corresponding author: e-mail: sivakumark78@gmail.com

**Keywords**: excess volume, excess isentropic compressibility, Redlich-Kister, FT-IR, DFT.

## Abstract

Densities (ρ) and speed of sound (u) have been experimentally determined for the binary mixtures of chlorobenzene with o-cresol, m-cresol and p-cresol as a function of temperature range from 303.15 to 313.15 K and at atmospheric pressure. The measured data of all the liquid mixtures was used to compute excess volume ($V^E$), isentropic compressibility ($k_s$) and excess isentropic compressibility ($k_S^E$). The calculated excess parameters have been fitted tothe Redlich-Kister and Hwang polynomial equations and the results were analyzed in terms of molecular interactions and structural effects between component molecules. Further, the measured data were also analyzed with Fourier transform infrared (FT-IR) spectroscopy since FT-IR is a powerful tool to get information regarding the existence of molecular interactions in binary liquid mixtures and by adopting the DFT/B3LYP/6–311++ G (d, p) level of theory to determine the optimized geometric structure of compounds chlorobenzene, o-cresol, m-cresol and p-cresol, as well as the complexes chlorobenzene + o-cresol, chlorobenzene + m-cresol and chlorobenzene + p-cresol.

# Excess thermodynamic study of binary mixtures of Benzyl alcohol with amides over entire miscibility range $(0 < x < 1)$ at temperature 298.15 - 323.15 K

K. Narendra[1],*, T. S. Krishna[2]

[1] Department of Physics, V R Siddhartha School of Engineering, SAHE, Vijayawada-520007, India
[2]Department of Physics, P B Siddhartha College of Arts & Science, Vijayawada-520010, India

*Corresponding author: narenk75@gmail.com

**Keywords**: Density; speed of sound; Benzyl alcohol; amides; intermolecular interaction

The speeds of sound, $u$ and densities, $\rho$, of the blends, of Benzyl alcohol with amides including those of pure liquids, have been determined from 0 to 0.1 mole fraction range of Benzyl alcohol with interval 0.1 at 298.15 - 323.15 K at pressure 0.1MPa. We used the measured data to assess the excess molar volumes, $V_{\mathrm{m}}^{\mathrm{E}}$, excess isentropic compressibility, $\kappa_{\mathrm{s}}^{\mathrm{E}}$, excess speeds of sound, $u^{\mathrm{E}}$, excess molar isentropic compressibility, $K_{\mathrm{s,m}}^{\mathrm{E}}$, excess isobaric thermal expansion, $\alpha_p^E$, were calculated and fitted with the Redlich-Kister equation. The excess partial molar volumes, $\bar{V}_{\mathrm{m},1}^{\mathrm{E}}$ and $\bar{V}_{\mathrm{m},2}^{\mathrm{E}}$ and excess partial molar isentropic compressibilities, $\bar{K}_{\mathrm{s,m},1}^{\mathrm{E}}$ and $\bar{K}_{\mathrm{s,m},2}^{\mathrm{E}}$, excess partial molar volumes, $\bar{V}_{\mathrm{m},1}^{\circ\mathrm{E}}$ and $\bar{V}_{\mathrm{m},2}^{\circ\mathrm{E}}$ and excess partial molar isentropic compressibilities, $\bar{K}_{\mathrm{s,m},1}^{\circ\mathrm{E}}$ and $\bar{K}_{\mathrm{s,m},2}^{\circ\mathrm{E}}$ of the components at infinite dilution have also been measured. The departure of measured properties has been explored in terms of intermolecular interactions.

**References**

[1] Mohammed Taghi Zafarani-Moattar, Hemayat Shekaari. J. Chem. Thermodyn., 38 (2006) 1377–1384.
[2] J. Pandurangarao, K. Narendra, V. Vishalakshma, T. S. Krishna, G. Srinivasa Rao, J. Chem. Thermodyn., 190(2024) 107222.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

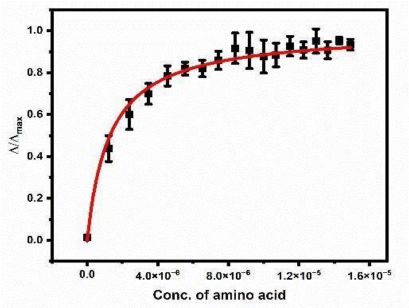
# Adsorption of Amino Acid on Gold Nanoparticles: A Thermodynamic Study

**PINKI MAHUR[1], KAMINI MISHRA*[2]**
Department of Chemistry, School of Advance Science (SAS)
Vellore Institute of Technology, Vellore
Corresponding author e-mail ID: kamini.mishra@vit.ac.in

**Keywords**: Adsorption, dynamic light scattering, Langmuir isotherm, binding constant, Gibbs free energy

The interaction of amino acids with gold nanoparticles (AuNPs) has significant implications in biomedicine, catalysis, and nanotechnology [1]. We investigate the adsorption of amino acids on AuNPs using dynamic light scattering (DLS), zeta potential, and absorption spectroscopy. In this study, we have chosen four categories of amino acids based on their side chain properties: positively charged, negatively charged, neutral, and thiol (SH)-containing small molecules. We have used a fixed amount of 15 nm citrate-capped AuNPs and added different amounts of amino acids to it. The AuNP-amino acid conjugates were then characterized by monitoring the changes in the hydrodynamic diameter and zeta potential as a function of amino acid concentration. We have extracted the binding constant ($K_b$) and Gibbs free energy ($\Delta G^\circ$ ) by using the Langmuir adsorption model [2].

We found that the thiol-containing small molecules exhibited the highest $K_b$ and $\Delta G^\circ$ values, followed by positively charged, neutral, and negatively charged amino acids. This could be because of strong covalent-like interactions with AuNP surfaces in the case of amino acids containing thiol side chains. Positively charged amino acids are mostly driven by electrostatic attractions, while neutral amino acids show moderate binding due to weaker non-covalent interactions. Negatively charged amino acids display the lowest binding affinity, reflecting hindrance due to electrostatic repulsion. These results underscore the pivotal role of side chain properties in amino acid-AuNP interactions, providing a foundation for tailoring nanoparticle functionalization in biomedical and nanotechnological applications.



**References:**
[1] Chakraborty, A., Boer, J. C., Selomulya, C., & Plebanski, M. *Bioconjugate Chemistry*, *29*(3) (**2017**) 657-671.
[2] Mishra, A., Mishra, K., Bose, D., Chakrabarti, A., & Das, P. K. *Physical Chemistry Chemical Physics*, 23(42) **(2021)** 24365-24376.

18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024

# Carbon dioxide capture with ionic liquids and deep eutectic solvents: a new generation of sorbents

**ARDILA H. TIWIKRAMA***, SALAL H. KHUDAIDA

Chemical Engineering and Biotechnology Department, National Taipei University of Technology, 1, Zhong-Xiao E. Road, Section 3, Taipei 10608, Taiwan
*Corresponding author: e-mail: ardilahayu@mail.ntut.edu.tw

**Keywords**: $CO_2$; ionic liquids, deep eutectic solvents; polyols; PC-SAFT

The high energy and cost requirements associated with $CO_2$ absorption from flue gasses represent a significant obstacle to large-scale applications. The development of a technically and economically efficient technology for $CO_2$ absorption is therefore essential. The inherent advantages of ionic liquids (ILs) in $CO_2$ capture have led to them being proposed as a potential alternative to conventional sorbents. As a result, interest has increased in the chemical modification of ILs to improve their $CO_2$ absorption capacity. As a new generation of ILs, deep eutectic solvents (DESs) are being investigated as more cost-effective alternatives to conventional ILs that exhibit high viscosity. The $CO_2$ absorption potential of functionalized DESs and ILs is investigated in this study [1,2]. The absorption capacity of ILs can be improved by incorporating $CO_2$-philic functional groups, such as amine, into the cation and/or anion component. In general, the anion component of ILs is functionalized more efficiently than the cation component. DESs have favorable solvent properties and the ability to capture $CO_2$, but their research is limited and underdeveloped compared to that of ILs. The solubility of $CO_2$ in diisoporpylethylammonium-based ILs and polyol-based DESs consisting of choline chloride (ChCl)/diethylene glycol (DEG), ChCl/triethylene glycol (TEG) and ChCl/tetraethylene glycol (TTEG) with a 1:4 molar ratio was determined using a variable volume high pressure cell at temperatures from 298.15 to 373.15 K and pressures up to 7 MPa [3]. The PC-SAFT strategy was used to correlate the experimental vapor-liquid equilibrium (VLE) data. In this study, the pseudo-pure components are referred to as ILs and DESs by fitting the PC-SAFT parameters to the density data of the pure ILs and DESs. The analysis has shown that the solubility of $CO_2$ in diisoporpylethylammonium-based ILs and polyol-based DESs is accurately characterized by the PC-SAFT equation of state. It is conceivable that novel ILs and DESs with encouraging absorption capacities can be developed.

**References**

[1] Tiwikrama, A. H., Khudaida, S. H., Long, C. H., *J. Chem. Eng. Data* 68 **(2023)** 3298.
[2] Tiwikrama, A. H., M.Taha, and M.J.Lee, *J. Taiwan Inst. Chem. Eng.* 112 **(2020)** 152.
[3] Chiu, H. Y., Lin, H. M., and Lee, M. J. *J. Supercrit. Fluids,* 82 **(2013)** 146.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# An updated Review on the Application of Nanofluids in several types of Heat Transfer Devices

**BRAJESH KUMAR AHIRWAR[1]*, ARVIND KUMAR[2]**
[1,2]Department of Mechanical Engineering, Maulana Azad National Institute of Technology, Bhopal
Madhya Pradesh 462003, India
*Corresponding author: e-mail: ahirwarbrajeshkumar@gmail.com

**Keywords**: Heat exchanger, Nanofluids, Nanoparticles, Volume fraction, Heat transfer

**Abstract:**

Since the idea of distributing nano particles into a fluid was first proposed in the latter half of the 20th century, the field of nanofluids has attracted considerable attention. This is demonstrated by the rise in the number of studies on nanofluids that are published each year. The main reasons for the growing interest in nanofluids are their improved thermophysical characteristics and their adaptability to a variety of thermal applications, such as solar energy harvesting for renewable energy production or improving the efficiency of heat exchangers used in industry. This article reviews the advancements achieved in the preparation of nanofluids and their applications in a range of heat transfer devices, including heat exchangers, solar collectors, refrigeration systems, radiators, thermal storage units, and electronic cooling. The efficiency and capacity of the solar energy storage and heat exchanger system can be improved by the use of nanofluids. In addition to providing readers with an update on current developments, this review will also address the future prospects and challenges facing nanofluids as the next generation of heat transfer fluids. Ultimately, an assessment of the benefits and drawbacks of nanofluids is provided, along with suggestions for more research that could spur the quick commercialization of nanofluids.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Formulation of Nanofluids based on Natural Deep Eutectic Solvents

**HRISHIKESH SARMA[1]*, TAMAL BANERJEE[1]**

[1]Department of Chemical engineering, IIT Guwahati, Guwahati 781039, India
*Corresponding author: e-mail: sarmahrishikesh199@gmail.com

**Keywords**: Deep Eutectic Solvents, Nanofluid, Thermal conductivity, Specific heat

Today, an array of strategies is being explored and evaluated to determine the optimal approach for enhancing the productivity of heat transfer fluids, with a particular focus on nanofluids. Deep eutectic solvents (DESs) especially Natural Deep Eutectic Solvents (NADESs) have emerged as promising materials poised to address the needs for sustainable ecological processes and to unlock avenues for surmounting the constraints of traditional fluids. This study introduces the synthesis and analysis of novel nanofluids formulated from NADESs. These NADESs comprise Betaine (Be) as a Hydrogen Bond Acceptor (HBA) with Lactic acid (LA) and Ethylene glycol (EG) as Hydrogen Bond Donors (HBDs). In this work, nanofluids are prepared using ratios with Be: LA (molar ratio of 1:2) (NADES1) and Be: EG (molar ratio of 1:4) (NADES2).

Functionalized multi-walled carbon nanotube (MWCNT) nanoparticles are then dispersed within these solvents. Properties such as thermal conductivity, specific heat capacity, density, and mass loss were measured and analyzed before and after the dispersion of nanoparticles. The results showed that the onset temperature for mass loss is 20-25°C higher in nanofluid prepared from NADES1 whereas the onset temperature was about 5°C lower than its base fluid NADES2.This shows that the addition of nanoparticle has led to increase in thermal stability in nanofluid prepared from NADES1 and decrease in thermal stability in nanofluid prepared from NADES2. The thermal conductivity of both the nanofluids was almost 7-9% higher (0.21-0.25 W/m.K) than that of the base fluid, and with an increase in the volume fraction (0.01-0.05) of the nanoparticle, there was an increase in thermal conductivity. The increase in thermal conductivity has resulted in increase in thermal stability as well as increase in energy efficiency of the nanofluid. It was observed that the nanofluids offer enhanced thermal conductivity and heat transfer properties as compared to base fluids. With NADESs as base fluid, they are poised to drive innovation while reducing environmental footprint and enhancing sustainability.

**References**

[1] S.U.S. Choi, *J. Heat Transf.*, 131 (3) (**2009**), 033106–033106-033109.
[2] H. Ghasemi, G. Ni, A.M. Marconnet, J. Loomis, S. Yerci, N. Miljkovic, G. Chen, *Nat. Commun*., 5 (**2014**) 4449.
[3] Dehury, P., Mahanta, U., Singh, R. and Banerjee, T.,*Journal of Molecular Liquids, 379*, (**2023**) 121700.

*18th International Congress on Thermal Analysis and Calorimetry,IITMadras, India,02-07 Sept. 2024*

# Investigation of phase equilibria on LiCl-$LaCl_3$ binary system

**P. PURKAIT[1], S. GHOSH[2], T.M. AMBIKA[2], C. ROUTRAY[2], R. SUDHA[2], R. GANESAN[2,3]***

[1]Reactor Facilities Group, [2]Materials Chemistry and Metal Fuel Cycle Group, [3]Homi Bhabha National Institute, Indira Gandhi Centre for Atomic Research, Kalpakkam, Tamil Nadu- 603 102, India
*Corresponding author: rajesh@igcar.gov.in

**Keywords**: Pyrochemical reprocessing, binary phase diagram, DTA, XRD

Molten LiCl-KCl eutectic is used as the liquid electrolyte medium in the pyrochemical reprocessing of spent metallic fuel. It is known as electrorefining process [1]. In this process, spent metallic fuel is anodically dissolved in the LiCl-KCl melt and fuel elements like uranium and plutonium are selectively electrodeposited at the cathodes leaving the fission product in the melt. Lanthanum is one of the major fission products [2]. In order to understand the interaction of $LaCl_3$ with LiCl-KCl melt, LiCl-KCl-$LaCl_3$ ternary phase diagram is being investigated. LiCl-$LaCl_3$ is one of the constituent binary diagrams. Hence, LiCl-KCl binary phase diagram investigation is taken up in author's laboratory by differential thermal analysis (DTA) and X-ray diffraction (XRD) methods.

LiCl and $LaCl_3$ are hygroscopic in nature. Hence, samples for DTA and XRD were prepared by mixing high pure LiCl and $LaCl_3$ inside an inert atmosphere glove box. Homogenised samples were studied for DTA by Setsys Evolution 16/18 equipment from 350°C to 900°C with controlled heating and cooling rates. Further, equilibrated samples at 450°C were loaded in specially designed sample holder and analyzed by XRD using CuKα radiation.

The DTA traces of all the sample mixtures showed sharp endothermic and concordant event at 490°C followed by a tail end which is attributed to liquidus temperature. The liquidus temperature of the samples decreased monotonically from the LiCl corner with the addition of $LaCl_3$. It reached a minimum and increased monotonically at the $LaCl_3$ rich corner. It is an indication of simple binary eutectic reaction. Further, LiCl and $LaCl_3$ were identified as coexisting solid phases in XRD. Hence, LiCl-$LaCl_3$ phase diagram is a simple eutectic binary system. The binary eutectic temperature was determined at 490 ± 5°C and its composition was arrived at 77.5mol% of LiCl and 22.5mol% of $LaCl_3$.

**References**

[1] J.J. Laidler, J.E. Battles, W.E. Miller, J.P. Ackerman and E.L.Carls, *Prog Nucl Energ,* 31(**1997**)131.
[2] E.A.C. Crouch, *Atom Data NuCl Data,* 19 (**1977**) 417.

**T1- OP 39**

# Thermo-Hydraulic Behavior of Non-Newtonian Fluids in Mixed Convection within an Open-Boundary Square Duct Featuring an Embedded Adiabatic Block

**Shantanu Dutta**[1*],**Aranyak Chakravarty**[2] , **MdNaim Hossain**[3] , **Koushik Ghosh**[4]

[1*] Department of Mechanical Engineering, Sanaka Educational Trust Group of Institutions
[2] School of Nuclear studies, Jadavpur University, Kolkata
[3] Department of Mechanical Engineering, Jalpaiguri Government Engineering College,
[4]Department of Mechanical Engineering, Jadavpur University, Kolkata
*Corresponding Author's Email: shantanudut@gmail.com

In this numerical work, we present numerical simulation of the flow characteristics and the heat transfer mechanism of a non-Newtonian power law fluid in an annular space between a central square adiabatic block and a square enclosure with open boundaries on bottom left and top right as well( see Fig 1). The aspect ratio of the adiabatic block of size L=0.2 of the dimensionless distance is maintained. The power-law index n is varied from 0.6 to 1.3. Prandtl number (Pr) is chosen to be 10 and the Reynolds (Re) varies from 100 to 300 while the Richardson number(Ri) is varied from Ri=0.01 to 5. The governing equations are solved using mixed finite elements method. The effects of the different parameters on the heat transfer and on the flow are examined. It is observed that streamlines and isotherm change in pattern with the change of power-law index at Ri=1 and 5 and the amount of the alteration increased for Pseduo plastic case(n<1). Nu increase with the augmentation of Re but not for n. The dimensionless average Nusselt number($\overline{Nu}$) escalation was observed when Re augmented from 100 to 300 and the rise of power-law index decreases the effect of heat transfer for different Ri.

**Keywords**: *Non-Newtonian fluid; Mixed Convection; Heat Transfer; Power law fluids.*

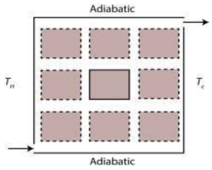


Fig 1: schematic of the enclosure

**References**

[1] Kefayati, G.R., 2014. Mixed convection of non-Newtonian nanofluids flows in a liddriven enclosure with sinusoidal temperature profile using FDLBM. *Powder technology*, *266*, (2014) pp.268-281.

[] Turan, O., Sachdeva, A., Chakraborty, N. and Poole, R.J., 2011. Laminar natural convection of power-law fluids in a square enclosure with differentially heated side walls subjected to constant temperatures. *Journal of Non-Newtonian Fluid Mechanics*, *166*(1718),(2011) pp.1049-1063.

18th International Congress on Thermal Analysis and Calorimetry,IITMadras, India,02-07 Sept. 2024

# Investigation of phase equilibria on LiCl-$LaCl_3$ binary system

**P. PURKAIT**[1], **S. GHOSH**[2], **T.M. AMBIKA**[2], **C. ROUTRAY**[2], **R. SUDHA**[2],
**R. GANESAN**[2,3]*

[1]Reactor Facilities Group, [2]Materials Chemistry and Metal Fuel Cycle Group, [3]Homi Bhabha National Institute, Indira Gandhi Centre for Atomic Research, Kalpakkam, Tamil Nadu- 603 102, India
*Corresponding author: rajesh@igcar.gov.in

**Keywords**: Pyrochemical reprocessing, binary phase diagram, DTA, XRD

Molten LiCl-KCl eutectic is used as the liquid electrolyte medium in the pyrochemical reprocessing of spent metallic fuel. It is known as electrorefining process [1]. In this process, spent metallic fuel is anodically dissolved in the LiCl-KCl melt and fuel elements like uranium and plutonium are selectively electrodeposited at the cathodes leaving the fission product in the melt. Lanthanum is one of the major fission products [2]. In order to understand the interaction of $LaCl_3$ with LiCl-KCl melt, LiCl-KCl-$LaCl_3$ ternary phase diagram is being investigated. LiCl-$LaCl_3$ is one of the constituent binary diagrams. Hence, LiCl-KCl binary phase diagram investigation is taken up in author's laboratory by differential thermal analysis (DTA) and X-ray diffraction (XRD) methods.

LiCl and $LaCl_3$ are hygroscopic in nature. Hence, samples for DTA and XRD were prepared by mixing high pure LiCl and $LaCl_3$ inside an inert atmosphere glove box. Homogenised samples were studied for DTA by Setsys Evolution 16/18 equipment from 350°C to 900°C with controlled heating and cooling rates. Further, equilibrated samples at 450°C were loaded in specially designed sample holder and analyzed by XRD using CuKα radiation.

The DTA traces of all the sample mixtures showed sharp endothermic and concordant event at 490°C followed by a tail end which is attributed to liquidus temperature. The liquidus temperature of the samples decreased monotonically from the LiCl corner with the addition of $LaCl_3$. It reached a minimum and increased monotonically at the $LaCl_3$ rich corner. It is an indication of simple binary eutectic reaction. Further, LiCl and $LaCl_3$ were identified as coexisting solid phases in XRD. Hence, LiCl-$LaCl_3$ phase diagram is a simple eutectic binary system. The binary eutectic temperature was determined at 490 ± 5°C and its composition was arrived at 77.5mol% of LiCl and 22.5mol% of $LaCl_3$.

**References**

[1] J.J. Laidler, J.E. Battles, W.E. Miller, J.P. Ackerman and E.L.Carls, *Prog Nucl Energ,* 31(**1997**)131.
[2] E.A.C. Crouch, *Atom Data NuCl Data,* 19 (**1977**) 417.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Study on Heat Capacity of Nickel-Titanium-Copper Shape Memory Alloys

**R SANTHOSH[1]*, K GURUVIDYATHRI[2], KOPPOJU SURESH[3]**
1DRDO Young Scientists' Laboratory for Smart Materials (DYSL-SM),
Defence Research and Development Organization (DRDO), Hyderabad, India.
2School of Engineering Sciences and Technology, University of Hyderabad, Hyderabad, India.
3International Advanced Research Centre for Powder Metallurgy and New Materials (ARCI),
Hyderabad, India. *Corresponding author: e-mail: santhoshr.dysl-sm@gov.in /
rsanthosh0112@gmail.com

**Keywords**: Heat Capacity, DSC, Ni-Ti-Cu, Shape Memory Alloy

Nickel-Titanium-Copper (Ni-Ti-Cu) shape memory alloys exhibit better functional stability due to the reduced thermal hysteresis [1]. In recent times, new alloy compositions with improved cyclic stability and actuation strain are identified through machine learning [2]. The thermodynamic properties of these alloy compositions are not available, to the best of our knowledge. Thermodynamic properties like heat capacity forms the basis for Gibbs energy models which could be used in computations for alloy engineering. The experimental data on heat capacity of unexplored compositions would augment the present thermodynamic descriptions of Ni-Ti-Cu system [3]. Hence, this study is carried to gather information on heat capacity at constant pressure ($C_p$) of the Ni-Ti-Cu alloy compositions through Differential Scanning Calorimetry (DSC) measurements. The $Ni_xTi_yCu_z$ ($32 \leq x \leq 47$, $40 \leq y \leq 52$, $3 \leq z \leq 21$; in *atom percent*) alloys are prepared through vacuum arc melting under flowing argon atmosphere. The alloy buttons are re-melted four times and heat treated in vacuum sealed quartz tubes and water quenched. The phases present in the alloys are identified through X-Ray Diffraction (XRD) analysis. The microstructure and chemical composition are analysed using Scanning Electron Microscopy (SEM) with Energy Dispersive Spectroscopy (EDS). The heat capacity of alloy compositions is measured through heat-flux type DSC using 3-step method at 10 K min$^{-1}$ with $\alpha$-$Al_2O_3$ standard for heat-flux calibration. The DSC traces (Fig.1a) shows that the alloys undergo a single step phase transformation of Martensite ⇌ Austenite during heating and cooling. The transformation of Martensite ⇌ Austenite is associated with latent heat typical to that of a first order transformation. The heat capacity is estimated from both heating and cooling cycles (Fig. 1b). The heat capacity of the alloys is analysed in comparison with the recent CALPHAD assessment of Austenite (A) and Martensite (M) phases in Ni-Ti-Cu system.

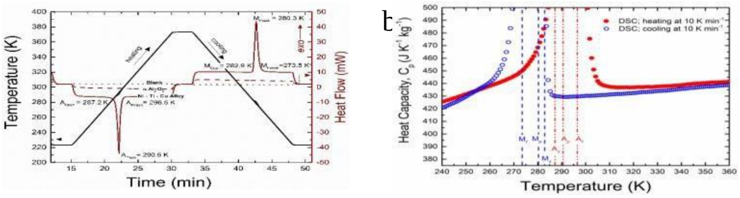


Fig. 1a: DSC traces of $Ni_{32}Ti_{48}Cu_{20}$ alloy along with that of $\alpha$-$Al_2O_3$ calibrant and blank run & Fig. 1b: Estimated heat capacity (latent heat contribution included) from heating and cooling cycles.

## References

[1] R. Zarnetta, P J S. Buenconsejo, A. Savan, S. Thienhaus, A. Ludwig *Intermetallics* 26 (2012) 98.
[2] W. Trehern, R. Ortiz-Ayala, K.C. Atli, R. Arroyave and I. Karaman *Acta Materialia* 228 (2022) 117751.
[3] A Povoden-Karadeniz, D C Cirstea and E Kozeschnik *IOP Conf. Ser.: Mater. Sci. Eng.* 123 (2016) 012038.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Sustainable Transformation: Green Synthesis of Reduced Graphite Oxide via Thermal Reduction

**PRAMOD RANJAN DASH[1], RITIKA JENA[2], BISWAJIT DALAI [1*], CHHATRAPATI PARIDA[2*]**

[1]Department of Physics, School of Sciences, Gandhi Institute of Engineering & Technology (GIET) University,
Gunupur 765022, India
[2]Department of Physics, Odisha University of Agriculture & Technology (OUAT), Bhubaneswar 751003, India
*Corresponding authors: e-mail: pramodranjan.dash@giet.edu ; biswajit@giet.edu ; sivaji_1976@yahoo.co.in

**Keywords**: Thermal analysis, green synthesis, XRD and Raman spectra, TGA, dielectric properties

The current study employs the Hummers method to obtain graphene oxide (GO) from graphite. The GO was subsequently exposed to heat in a muffle furnace at a temperature of 600°C for 20 minutes and 1 hour, resulting in the production of thermally reduced GO, also known as TRGO. The TRGO was analyzed using XRD, FTIR, Raman spectroscopy, and DTGA / TGA to identify the specific changes caused by the heat treatment. The transformation from 3D GO to 2D graphene was assessed by examining alterations in the G peak in TRGO and the 2D Raman peak. The Raman and XRD spectra are utilized to examine the influence of thermal irradiation on the dimensions of crystallites and the separation between crystal planes. The characterization results demonstrate the elimination of several oxygen-containing functional groups from GO upon exposure to thermal radiation, showing a molecular interaction between GO and thermal energy. A thermogravimetric analysis (TGA) was performed on graphite, oxidized graphite, and TR GO to investigate their thermal degradation mechanism and thermal stability up to 600$^0$C. The dielectric properties of TR GO were evaluated and compared to those of graphite and GO, including the real component of the dielectric constant, dielectric loss, and AC conductivity in the frequency range spanning from 4Hz to 4MHz and the temperature range ranging from ambient temperature to 130°C. The Cole-Cole graph analysis was employed to observe their non-Debye-type relaxation behavior.

## References

[1] Sahoo, D. kumar, Dalai, B., Dash, S., & Parida, C. A new perception to the spectroscopic, dielectric and impedance behavior of graphene oxide. Ferroelectrics, 603(2023) 185–209. https://doi.org/10.1080/00150193.2022.2159231.

[2] Sahoo, D. K., Dalai, B., Mohanty, A. K., & Parida, C. Novel approach for modification of graphene oxide using continuous wave-laser obtained from surgical laser diode. Radiation Effects and Defects in Solids, 179 (2024) 738-761. https://doi.org/10.1080/10420150.2024.2309199.

[3] Dalai B, Patra B, Das N, Sahoo R, Sahoo DK, Parida C, Dash SK. Synthesis, Characteristics and Applications of Graphene Composites: A Survey. JOTCSA. 10(2023) 757-72. https://doi.org/10.18596/jotcsa.1234196

# Investigation of porous metal foam enhanced PCM-based BTMS for CubeSat applications

**SAUKHYA TELGE[1]***

[1]Department of Mechanical Engineering, Indian Institute of Technology Bombay, Maharashtra-400076, India
*Corresponding author: e-mail: 210100135@iitb.ac.in

**Keywords**: BTMS, PCM, CubeSat, porous medium

CubeSats are nanosatellites of standard sizes and form factor. Due to their many advantages, such as low development and launch costs, there has been a surge in the number of CubeSats being launched yearly [1]. However, the CubeSat form factor comes with its own disadvantages, one of which is the high heat dissipation in a small volume, leading to the need for a good thermal control system. Due to the limited power availability in CubeSats, passive thermal control methods are generally preferred. One such passive thermal control method is Phase Change Materials (PCM).

This paper studies the application of a PCM-based Battery Thermal Management System (BTMS) for satellites of the CubeSat form factor. Since weight is a constraint in all space missions, especially in CubeSats, efforts are made towards minimising the weight of the BTMS while maintaining the thermal performance. To this extent, the PCM is embedded in porous metallic foam and its performance is examined. The metallic porous medium not only reduces the weight of the BTMS but also enhances the thermal conductivity and uniformity of heat distribution within the PCM [2]. Numerical simulations are performed to analyse the battery temperatures in orbit with and without the proposed BTMS.

**References**

[1] Shiroma, W.A., Martin, L.K., Akagi, J.M. et al. CubeSats: A bright future for nanosatellites. cent.eur.j.eng 1, 9–15 (2011). https://doi.org/10.2478/s13531-011-0007-8

[2] Mohamed Moussa EL IDI, Mustapha KARKRI, Manel KRAIEM, Preparation and effective thermal conductivity of a Paraffin/ Metal Foam composite, Journal of Energy Storage, Volume 33, 2021, 102077, ISSN 2352-152X, https://doi.org/10.1016/j.est.2020.102077.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Experimental Study of Natural Convection Heat Transfer in Horizontal Fin Arrays

**RAJAMOHAN GANEASN*, KRISHNAMANI SELVARAJ, PRAKASH DHAKSHINAMOORTHY,**

*School of Mechanical Engineering, SASTRA Deemed University, Thanjavur, Tamil Nadu, India*
*Corresponding author: rajamohan@mech.sastra.ac.in

## Abstract

The research aims to investigate experimentally the natural convection heat transfer through different fin designs for various engineering applications, such as heat exchangers, electronic equipment cooling, and related industrial applications to enhance heat transfer. Fins with the optimal geometry that corresponds to the maximum heat transfer rate should be employed when an array of fins is used to promote heat transfer under natural convection conditions, and it will ensure that this is compatible with available space and budgetary constraints. According to the literature, various fin patterns help to give a deeper understanding of heat transmission via natural convection. This experimental study provided correlations between fin spacing, Rayleigh number, and Nusselt number on the experimental data and guidelines for further developing heat exchangers. The experiment results reveal that higher temperatures appear for continuous fins than the interrupted and rubbed fins and a higher heat transfer coefficient and rate of Nusselt number appear for rubbed fins.

**Keywords**: Natural convection, Heat transfer, Experimental study, Interrupted Fins.

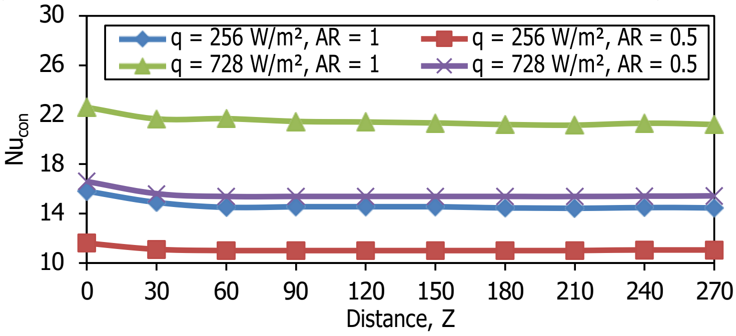


Fig. 1: Effect of average convective Nusselt number at the heated wall

### References

[1] S. Kiwan, H. Alwan and N. Abdelal, An experimental investigation of the natural convection heat transfer from a vertical cylinder using porous fins, Applied Thermal Engineering, 179 (2020) 1359.
[2] J.O. Okon, S.O. Effiom, Numerical simulation of the thermal performance of a wavy fin configuration for a straight fin array, Scientific African, 16, (2022) 1265.
[3] X. Meng, J. Zhu, X. Wei and Y. Yan, Natural convection heat transfer of a straight-fin heat sink, International Journal of Heat and Mass Transfer, Volume 123 (2018) P561-568.

*18th International Congress on Thermal Analysis and Calorimetry, IITMadras, India,02-07 Sept. 2024*

# Thermodynamic studies on Gd-Te system

**S SHYAM KUMAR[1]*, C.R. PATRA[1], R. GANESAN[1]**

[1]Materials Chemistry and Metal Fuel Cycle Group, Indira Gandhi Centre for Atomic Research,
Kalpakkam, Tamil Nadu- 603 102, India
*Corresponding author: shyam@igcar.gov.in

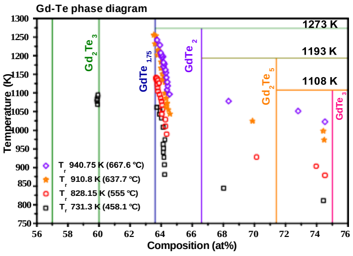
**Keywords**: Isopiestic, Fission products, FCCI, Rare earth, thermodynamic, intermetallic compounds

Nuclear fission results in the cascade of several fission products. Rare earth elements has a share of ~25% of the fission products. This investigations attempts to decipher the interactions of one of the rare earth fission product viz., gadolinium with tellurium. Formation of intermetallic compounds, would abate fuel clad chemical interactions (FCCI) [1]. In this context, investigation on Gd-Te system is carried out.

The experimental set up used for investigation is described elsewhere [2]. Experimental results of isopiestic experiments of Gd - Te system for reservoir temperatures of 731, 828, 910, 940 K is superimposed on the reported Gd - Te phase diagram [3] and is presented in Fig 1. The overall composition of the samples obtained from these experiments lie from 59 to 75 at % which lies from temperature 811 K and 1256 K.

It can be seen that the majority of the data were clustered in $GdTe_{1.75}$ and few of them in $Gd_2Te_3$ and $GdTe_3$ intermetallic compounds. Existence of non-stoichiometry in these compounds is evident from the distribution of the samples in the phase diagram.

Many samples are obtained in the two phase regions viz., $GdTe_2$ + $Gd_2Te_5$ and $Gd_2Te_5$ + $GdTe_3$. Thermochemical activity of Te was determined and the results related to it will be discussed and presented.



## References

[1] N.D. Jerred, R. Khanal, M.T. Benson, E. Perez, J.A. King, M. Dubey, J. Burns, I. Charit, S. Choudhury, R.D. Mariani, Evaluation of Tellurium as a Fuel Additive in Neodymium-Containing U-Zr Metallic Fuel, Sci. Rep. 9 (2019) 10643.

[2] S. Shyam Kumar, G. Rajendra Prasad, J.P. Rao, V. Suresh Kumar, R. Ganesan, V. Jayaraman, Design, Development, and Instrumentation of Isopiestic Experimental Setup, Rev. Sci. Instrum. 93 (2022) 44105.

[3] T.B. Massalski, H. Okamoto, P.R. Subramanian, L. Kacprezak, Binary Alloy Phase Diagrams, 2nd ed., ASM International, The Materials Information Society, Ohio, 1990.

*18th International Congress on Thermal Analysis and Calorimetry, IITMadras, India,02-07 Sept. 2024*

# Multifaceted Characterization of Zinc-Doped Chalcogenide Glasses: Unveiling the Impact on Thermal, Mechanical, and Electrical Properties

**VISHNU SARASWAT[1], NEERAJ MEHTA*[1],**

[1]Department of Physics, Institute of Science, Banaras Hindu University, Varanasi (221005), India
*Corresponding author: e-mail: dr_neeraj_mehta@yahoo.co.in

**Keywords**: thermal analysis, DSC, hardness, dielectric

This comprehensive study investigates the glass-to-crystal phase transformation in a novel chalcogenide glass system, Se-Te-Sn-Zn (STSZ). The researchers synthesized a series of STSZ glasses with varying Zn concentrations ($Se_{78-x}Te_{20}Sn_2Zn_x$, where x = 0, 2, 4, and 6) and conducted detailed thermal, structural, and electrical characterization.

The thermal analysis using Differential Scanning Calorimetry (DSC) reveals a significant increase in the crystallization rate upon adding Zn to the parent Se-Te-Sn glass. As the Zn content increases, the average heat of atomization and overall mean bond energy decrease, corresponding to a reduction in the cohesive energy of the samples. An inverse relationship is observed between the thermal stability parameter and the enthalpy released during the glass-to-crystalline phase transformation. The researchers also performed micro-indentation tests to evaluate the hardness and other mechanical properties, such as the modulus of elasticity, minimal micro-void formation energy, glass fragility index, and micro-void volume. The covalent nature of the glassy system was examined, and the fracture toughness and crack patterns were reported. Additionally, the study delved into the dielectric behavior, thermally activated a.c. conduction, and resistive switching properties of the STSZ glasses. The results indicate that the dielectric constant, dielectric loss, and a.c. conductivity is significantly influenced by the Zn concentration, with the a.c. conduction following the correlated barrier hopping (CBH) mechanism with bi-polaron hopping as the leading conduction mechanism. The resistive switching behavior is also found to be modified by the incorporation of Zn, which is explained using the chemically ordered network (CON) model and the heavy cross-linking of the glass matrix due to the isomers of $Se_yZn_y$ clusters.

Overall, this comprehensive study provides valuable insights into the glassto-crystal phase transformation and the associated physicochemical properties of the novel STSZ chalcogenide glass system, which can have important implications for various technological applications.

## References

[1] Y. Sun, Z. Sun, S. Gao, H. Cheng, Q. Liu, J. Piao, T. Yao, C. Wu, S. Hu, S. Wei, Y. Xie, *Nat Commun* 3 (**2012**) 1057.

[2] J. P. Dubey, R. Tiwari, K. S. Upadhyaya, P. K. Pandey,. *Turkish J. Phys*., 40 (**2016**) 201-208.

[3] S. Deb, P. K. Kalita, P. Datta, *Phys. Scr*., 95 (**2020**) 095810.

[4] V. Saraswat, S. K.Pal, A. Dahshan, and N. Mehta, *Journal of Non-Crystalline Solids, 617* (**2023**) 122487.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Investigating the Dynamics of Shock Wave and Flame Interactions

**SIDYANT KUMAR, CHIKMATH L[*], SOUJANYA P, RAHIL I.G, NIDHI N. M, MADHUSHREE P.**

Department of Aeronautical Engineering, KLS Gogte Institute of Technology, Belagavi-590008,
Karnataka, India
*Corresponding author: lokamanyachikmath@gmail.com

**Keywords**: Flame, Instability, Premixed combustion, Shock wave

The process of premixed combustion [1] is widely used in aerospace applications such as Ramjet combustion, anti-aircraft flare systems, and premixed gas turbines. The interaction of the shock wave with this premixed combustion flame is schematically shown in figure 1. scramjet combustion.

Fig. 1: Schematic of shock flame interaction in the cross-stream direction

Numerical simulation [2,3] are conducted to study the effect of shock waves on the Ethylene-air flame [4] in cross-flow configuration. The evolved related dynamics and flame propagation will be observed. The dynamics and evolution of the flame will be observed under varying shock strength ($\varepsilon = 0.5$, 1 and 1.5). Additionally, this analysis includes an examination of potential combustion instability through understanding the variation in dynamic pressure across the interaction zone. The structure of the shock wave will be captured using the numerical schlieren. The mixing of temperature and its temporal variation along the streamline direction of the shock wave is examined to justify the effectiveness of inducing turbulence due to impulsive aerodynamic loading.

## References

[1] Sherif S. Rashwan, Medhat A. Nemitallah, and Mohamed A. Habib; Review on Premixed Combustion Technology: Stability, Emission Control, Applications, and Numerical Case Study, Energy & Fuels 2016

[2] Ulrich Bielert,, Martin Sichel, Numerical Simulation of Premixed Combustion Processes in Closed Tubes, Combustion and Flame, 1998

[3] B.Rogg; Modelling and Numerical Simulation of Premixed Turbulent Combustion in a Boundary Layer; Proceedings of Turbulent Shear Flow 7, 1991

[4] Shinji Nakaya, Hajime Yamana and Mitsuhiro Tsue; Experimental investigation of ethylene/air combustion instability in a model scramjet combustor using image-based methods, Proceedings of the Combustion Institute, 2021

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Density, Speed of Sound, Refractive Index, FT-IR and computational studies of binary systems of ethyl lactate with 1-heptanol, 1-octanol, 1-nonanol at T = (298.15 – 323.15) K

**TAMMISETTY ANKAIAH[1], SREENIVASULU KARLAPUDI[2], KASIBHATTA SIVA KUMAR[3], NEELAM YUGANDHAR SREEDHAR[1*]**

[1]Thermophysical Laboratories, Department of Chemistry, Sri Venkateswara University, Tirupati-517502, Andhra Pradesh, India.
[2]Department of Chemistry, Sree Rama Engineering College, Tirupati-517507, Andhra Pradesh, India.
[3]Department of Chemistry, S.V. Arts college (T.T.D'S), Tirupati-517502, Andhra Pradesh, India.
*Corresponding author: e-mail: nysthermodynamic@gmail.com

**Keywords**: ethyl lactate, 1-alkanol, excess property, molecular interactions, FT-IR, DFT.

## Abstract

In the present work, we measured density (ρ), speed of sound (u) and refractive index ($n_D$) for three binary liquid mixtures of ethyl lactate with 1-heptanol, 1-ocatanol and 1-nonanol at temperature range from 298.15 to 323.15 K with interval of 5K and 0.1 MPa. Excess volume ($V^E$), isentropic compressibility ($k_s$), excess isentropic compressibility) ($k_S^E$) and excess refractive index ($n_D$) were calculated from experimental results and fitted to the Redlich-Kister polynomial equation. The results suggest that excess volume and excess isentropic compressibility data of three binary systems are positive over the whole composition range and increases with increasing the 1-alkanol chain length and temperature. Further, the excess refractive index values of all the binary liquid mixtures are negative over the entire composition range and decrease with increasing temperature. The type and extent of molecular interactions that are prevailing between ethyl lactate and 1-alkanol were further conformed by FT-IR spectral data and density functional theory (DFT).

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Enhancement of Heat Transfer with Spinel-Type Ferrite Magnetic Nanofluids Under External Magnetic Fields

**UMAMAHESWARI. S[1], MOORTHI PICHUMANI[1*]**

[1]Department of Nano Science and Technology, Sri Ramakrishna Engineering College,
Coimbatore-641022, India
*Corresponding author: e-mail: mpichumani@srec.ac.in

**Keywords**: Heat transfer enhancement, Magnetic nanofluid, Magnetic field, CFD

Nanofluids present a promising alternative to conventional coolants in heat transfer systems. Various nanomaterials, including metals, metal oxides, and carbon-based materials, are utilized for heat transfer applications [1]. Spinel-type ferrite nanoparticles, characterized by their superparamagnetic properties can be used to synthesize magnetic nanofluids [2]. The fluid velocity, thermal conductivity, and viscosity of these magnetic nanofluids can be regulated by applying external magnetic field [3]. This study examines the enhancement of the heat transfer rate in a shell and helically coiled tube heat exchanger using $MnFe_2O_4$ nanoparticles under magnetic field and compared to water, through CFD analysis. The average Nusselt number shows an increment up to 19% compared to water. The effect of volume fraction of nanoparticles on the heat transfer rate is investigated for 0.1 vol%, 0.5 vol%, 0.75 vol%, and 1 vol% with Reynolds number varying from 1000 to 6000. Using 1 vol% results in a 14% enhancement in heat transfer rate compared to 0.1 vol%. The maximum heat transfer rate of 5080.07 W is observed at Re=6000 for the magnetic nanofluid without magnetic field, while the presence of an external magnetic field with an intensity of 1000 G increased the heat transfer rate to 5242.55 W. A linear increase in heat transfer rate, overall heat transfer coefficient and effectiveness of the heat exchanger is observed for various Reynolds numbers and nanoparticle volume fractions. These ferrite based magnetic nanofluids also have extensive applications in heat sinks, heat pipes, and other fields such as biomedical, environmental, and electronic engineering [4].

**References**

[1] Wei, H., Moria, H., Nisar, K. S., Ghandour, R., Issakhov, A., Sun, Y., Kaood, A., and Youshanlouei, M. M. "*CASE STUD THERM ENG*, vol. 25, Jun. 2021.

[2] M. Amani, P. Amani, A. Kasaeian, O. Mahian, and S. Wongwises, *Mol Liq*, vol. 230, pp. 121–128, Mar. 2017.

[3] A. P. Avita, F. Fadel, P. Poppy, and S. Sukarni, *Key Eng. Mater*, Trans Tech Publications Ltd, 2020, pp. 38–46.

[4] I. Sharifi, H. Shokrollahi, and S. Amiri, *J MAGN MAGN MATER*, Mar. 2012.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermal Stability of monoethanaol amine based Deep Eutectic Solvent for Different Molar Ratio

**VICHITRA MALAIYARASAN[1], ANANTHARAJ RAMALINGAM[2*]**

[1]Sri Sivasubramaniya Nadar College of Engineering
[2]Chemical Engineering, SSN College of Engineering, Chennai, Tamil Nadu 603110, India,
*Corresponding author: e-mail: anatharajr@ssn.edu.in

**Keywords**: deep eutectic solvent; thermal stability; thermal gravimetric analysis (TGA); and differential scanning calorimetry (DSC)

In this study, the monoethanaol amine-based deep eutectic solvent was prepared at different mole ratios 1:2, 1:3, 1:4, 1:5, 1:6, and 1:7 and characterized their thermal stability in terms of decomposition temperatures, mass loss, and melting temperature by thermal gravimetric analysis (TGA) and differential scanning calorimetry (DSC). Here choline chloride acts as a hydrogen bond acceptor (HBA) and monoethanolamine as a hydrogen bond donor (HBD). It was observed that thermal stability was increased when the HBD increased. It was also noted that HBD plays a vital role in DES's thermal stability, which mainly depends on intermolecular interactions. Similarly, in DSC 1:6 and 1:7 high melting temperature and high enthalpy were observed compared to other mole ratios. It denotes that increasing the HBD ratio melting temperature also increased due to stronger intermolecular force and interaction between HBA and HBD in DES

## References

[1] F. S. Mjalli, G. Murshid, S. Al-Zakwani, A. Hayyan, Fluid Phase Equilib. 2017, 448, 30–40.
[2] J. Han, C. Dai, G. Yu, Z. Lei, *Green Energy Environ*. 2018.
[3] X. Li, K. H. Row, *J. Sep. Sci*. 2016, 39 (18), 3505–3520.
[4] A. Paiva, R. Craveiro, I. Aroso, M. Martins, R. L. Reis, A. R. C. Duarte, *ACS Sustain. Chem. Eng*. 2014, 2 (5), 1063–1071.

**T1- OP 51**

# Thermal Study of Advanced Phase Change Materials with Zinc as a Chemical Modifier

**VISHNU SARASWAT[1], NEERAJ MEHTA*[1],**

[1]Department of Physics, Institute of Science, Banaras Hindu University, Varanasi (221005), India
*Corresponding author: e-mail: dr_neeraj_mehta@yahoo.co.in

**Keywords**: thermal analysis, DSC, glass transition, specific heat

The thermal analysis conducted in this study aims to investigate the glass-to-crystal phase transformation in a newly synthesized glassy system, specifically SeTeSnZn alloys. This system comprises chalcogenides Se and Te as primary elements, with Sn as the third element in the parent alloy, and Zn as a chemical modifier. The impact of increasing Zn concentration at the expense of Se is analysed by correlating the kinetics of structural relaxation during the glass transition and devitrification during the crystallization phenomena in the chalcogenide glasses (ChGs) of the quaternary STSZ system [$Se_{78-x}Te_{20}Sn_2Zn_x$ $(0 \leq x \leq 6)$], along with their various physicochemical properties. A significant increase in the crystallization rate is observed following the addition of Zn to the parent SeTeSn glass. As the Zn content increases, both the average heat of atomization and overall mean bond energy decrease, corresponding to a reduction in the cohesive energy of the samples. An inverse relationship is noted between the thermal stability parameter and the enthalpy released during the glass-to-crystalline phase transformation. Furthermore, the study calculates composition-dependent specific heat, and entropy for the glass transition region, as well as examining thermal conductivity and thermal diffusivity.

## References

[1] Y. Sun, Z. Sun, S. Gao, H. Cheng, Q. Liu, J. Piao, T. Yao, C. Wu, S. Hu, S. Wei, Y. Xie, Fabrication of flexible and freestanding zinc chalcogenide single layers. Nat Commun 3 (2012) 1057.
[2] J. P. Dubey, R. Tiwari, K. S. Upadhyaya, P. K. Pandey,Crystal dynamics of zinc chalcogenides III: an application to ZnTe. Turkish J. Phys., 40(2016) 201-208.
[3] S. Deb, P. K. Kalita, P. Datta, Opto-electronic characterization of starch capped zinc chalcogenides (core-shell) nanocomposites and their application as Schottky device. Phys. Scr., 95 (2020) 095810.

# Thermophysical Properties Study on Composite Phase Change Material for Energy Recovery Applications

**SOLAIMALAI RAJA R, HASNA LOUAHLIA*, HAMID GUALOUS**
[1]University Laboratory of Applied Sciences of Cherbourg · LUSAC, University of Caen Normandy,
Site of Saint-Lo 50000, France
*Corresponding author: e-mail: hasna.louahlia@unicaen.fr

**Keywords**: Thermal property, Physical property, Composite phase change material,

The current study deals with the preparation and characterisation of composite phase change material (CPCM) for energy recovery applications. The CPCM is prepared via the melting cum blending method. To prepare CPCM, the carbon-based (CBM) porous (Porous Graphite (PG)) and non-porous materials (Graphite/Graphene) have been utilised, which were selected based on their favourable properties such as good porous structure and high thermal conductivity [1,2]. The CPCM contains a PCM with a phase change temperature of 23 °C and phase change enthalpy of ~200 J/g. The PCM is organic and hydrophobic in nature. Also, it has no supercooling effect and good cycling stability. After preparing the CPCM, thermo-physical properties such as thermal conductivity (KD2 thermal analyser), density (Pycnometer and gas pycnometer), Scanning electron microscopic analysis (SEM), phase change enthalpy (Differential scanning calorimeter(DSC)), thermogravimetric analysis (TGA), specific heat (Modulated DSC), Fourier Transform infrared spectroscopy (Infrared spectroscopy) were studied for PCM and CPCM. The novelty of the research work relied on preparing CPCM with desired thermo-physical properties to avoid stability (particularly achieving a suitable physical property; not investigated previously [2]) & low conductivity issues.

Further, FTIR results showed that PCM and CBM are chemically compatible with each other, and only physical interaction prevails between them. The inclusion of high thermal conductivity CBM enhances the thermal conductivity proportionally (16 to 20 times). At the same time, the phase change enthalpy of CPCM was decreased relative to the concentration of CBM (18% to 20%). The transient heat transfer study was performed, and it was found that the prepared CPCM can be effectively used for heat recovery and heat storage applications.

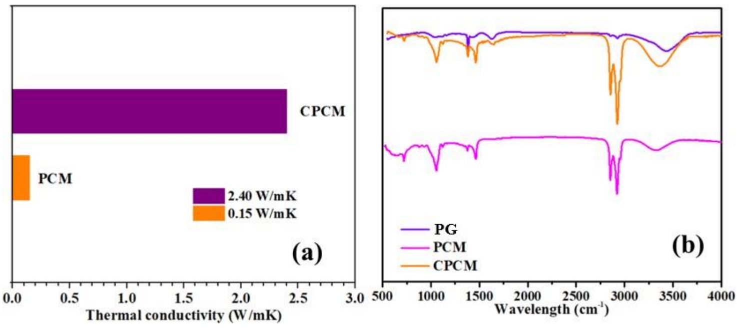


Fig.1 (a) Thermal conductivity and (b) FTIR results

## References

1. Chinnasamy V, Heo J, Jung S, Lee H, Cho H. Shape stabilised phase change materials based on different support structures for thermal energy storage applications–A review: Energy, 125463.
2. Zhang Y, Jia Z, Moqeet Hai A, Zhang S, Tang B. Shape-stabilization micromechanisms of form-stable phase change materials-A review. Compos Part A Appl Sci Manuf 2022;160:107047.

**T1- OP 53**

# HEAT TRANSFER AND ENTROPY GENERATION IN A HEAT EXCHANGER TUBE CARRYING DOUBLE PERFORATED TWISTED TAPE WITH V-WINGLETS

**BIPIN KUMAR[1*], ANIL KUMAR PATIL[1], MANOJ KUMAR[1]**

[1] Department of Mechanical Engineering, DIT University, Dehradun 248009, India
[*]Corresponding author email: bipin.kumar@dituniversity.edu.in

**Keywords**: Twisted tape, Twist ratio, V-winglet, Nusselt Number, Friction Factor, Reynolds number, Entropy generation

Twisted tape is a swirl producing insert which creates co-swirl and counter-swirl fluid motion in a heat exchanger tube. The present experimental work investigates the effect of V-winglet in double perforated twisted tape (DPTT) with co-swirl (CO) and counter swirl (COT) orientations on thermal performance and entropy generation of a tubular heat exchanger. During the experimental data collection, the Reynolds number (Re) is varied in the range of 10400 – 22800 and the twist ratio (y) of insert is varied from 2 to 6. The experiments are also performed for single solid twisted tape (STT) and perforated twisted tape (PTT) under similar operating conditions. The maximum enhancement in the Nusselt number is found to be 2.62 for DPTT-COT (V-winglet, y: 2). However, the highest thermal performance factor of 1.69 is attained by DPTT-COT (V-winglet, y: 4). The minimum value of entropy generation number ($N_s$) corresponds to the DPTT-COT (V-winglet, y: 6).

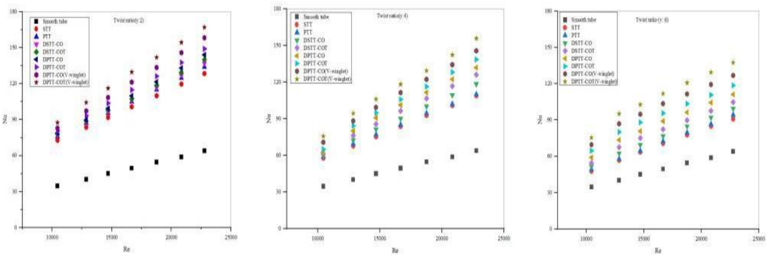


Fig. 1: Variation of Nusselt number vs Reynold number for different inserts

## References

[1] S. Eiamsa-ard, C. Thianpong, and P. Promvonge, *Int. Communication in Heat Mass Transfer*, 33 (**2006**) 1225–1233.

[2] P. Promvonge, *Energy Conversion and Management*, 49 (**2008)** 29492955.

[3] M.M.K. Bhuiya, M.S.U. Chowdhury, M. Saha, M.T. Islam, *International Communications in Heat and Mass Transfer* 46 (**2013**) 49–57.

[4] B. Kumar, M. Kumar, A. K. Pati, & S. Jain, *Experimental Heat Transfer*, 32:6, (**2019**) 524-544.

[5] Eiamsa-ard, W. Changcharoen, R. Beigzadeh, P. Eiamsa-ard, K. Wongcharee, V. Chuwattanakul, *Chemical Engineering and Processing - Process Intensification*, 160:108304 (**2021**).

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Longitudinal Vortex Generation using Various Winglet Configurations in Double-Pipe Heat Exchangers

**AMOGH S AMBLIHALLI[1]*, H M UMA MAHESHWARA URF ABHISHEK[1], DRUVA MURALI[1], HET MILIND AMBANI[1], B VANIRUDH KASHYAP[1], DR. RAJENDRA PRASAD[2]** AND DR. V. KRISHNA[1]***

[1]Department of Mechanical Engineering, PES University, Bangalore, Karnataka, India
[2]Department of Mechanical Engineering, Manipal Institute of Technology, Bangalore, Karnataka, India
*Corresponding author: e-mail: aamblihalli@gmail.com

**Keywords**: thermal analysis, longitudinal vortex generation, heat exchanger, winglet

Vortex generators provide an effective and passive method of improving heat transfer by delaying flow separation and generating turbulence in fluid. Previous studies have focused on using wings and winglets of delta and rectangular shapes for fin-and-tube heat exchangers, pipes, etc. They have also shown that longitudinal vortex generation is one of the most effective methods to improve heat generation. The use of dimples and protrusions for vortex generation and improving heat transfer in pipes has also been done. This study delves into the computational simulation of the longitudinal vortex generation of the delta, rectangular and Wheeler winglet configurations in pairs, triplets and with dimples on the winglets in double-pipe heat exchangers. The outer pipe is made of ASTM 304 stainless steel and the inner pipe was made of copper. The numerical analysis was carried out by implementing the k-ω SST turbulence model. Parametric studies have been performed for a Reynolds number range of 4000-20000 for all models. It was observed that the maximum heat transfer characteristics were brought about by using rectangular winglet longitudinal vortex generators (RWLVG) in pair configuration. Maximum percentage increase of heat transfer rate was found to be in triangular winglet longitudinal vortex generators (TWLVG) in pair configuration at Re = 12,000 at 29.95%.

T1- OP 55

# Study of Inorganic carbonate-based flame-retardants for leather application: special focus on thermal characterization.

**ANSALIN GNANA SOWNDARYA A[1,2], SUJATA MANDAL [1,2]***

[1] Advanced Materials Laboratory (AML), CSIR – Central Leather Research Institute, Chennai-600020, India.
[2] Academy of Scientific and Innovative Research (AcSIR), Ghaziabad 201002, India
*Corresponding author: e-mail: sujata@clri.res.in, sujatamandal@rediffmail.com

**Keywords**: Thermal analysis, Leather, Inorganic carbonates, Flame retardants

Flame Retardant (FR) chemicals slow the start of a fire or its spread in case of fire accidents. During manufacturing, FR chemicals are added to furniture, electronics, building materials, fabrics, etc. Leathers are strong, durable, and flexible natural materials they find wide applications in protective garments, footwear, fashion garments, upholstery, accessories, etc. Incorporating FR chemicals into leathers is challenging. Thermal and calorimetric analysis plays a vital role in studying the potential and efficiency of FR chemicals.

Calcium carbonate (CC), and Magnesium Carbonate (MC) were selected for the present study and characterised using XRD, FTIR, particle size, and zeta potential. The potential of the selected FR chemicals was studied with the help of differential scanning calorimetry (DSC). The heat flow studies of FR chemicals help us understand the flame-retarding ability of them.

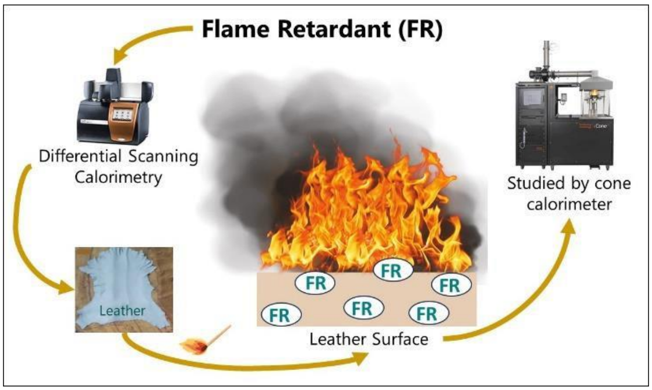


Fig. 1: Scheme of work

The selected FR chemicals were added to the leather (during the post-tanning operation, and the treated leathers were studied for improvement in Flame retardancy. The organoleptic properties of the FR-treated leathers were also studied. The total heat released (THR), peak rate of heat release (PHRR), average rate of heat release (AHRR), average effective heat of combustion (AEHC), and sample mass loss (SML) of the FR-treated leathers were analysed from cone calorimeter results.

**References:**

[1] Ansalin, G. S. A., Sujata, M., Prasanna, R., *Applied Clay Science*, 230 (2022) 106714.
[2] Budrugeac, P., Cucos, A., Miu, L., 2011. *J. Therm. Anal. Calorim.* 104, 439–450.
[3] ISO, 5660-1: 2015 Reaction-to-Fire Tests, 2015.

*18th International Congress on Thermal Analysis and Calorimetry, IITMadras, India,02-07 Sept. 2024*

# Modeling and Efficiency Analysis of SCO2 Recompression Cycle with Axial Flow Turbine Using Aspen HYSYS

**GARIMA BHARTI**[1]*, MANJUNATH K[2], ANIL KUMAR[3]

[1,2,3]Department of Mechanical Engineering, Delhi Technological University, Delhi 110042, India
*Corresponding author: garimabharti_2k21phdme13@dtu.ac.in

**Keywords**: Axial flow turbine, $SCO_2$, Recompression cycle, Aspen Hysys, Efficiency

The $SCO_2$ recompression cycle features low complexity and compact turbomachinery compared to conventional cycles. Although advanced high-power cycles present challenges and have yet to be widely implemented, this study focuses on incorporating an axial flow turbine into a $SCO_2$ recompression cycle, marking a step towards advancement. The modeling is conducted using Aspen HYSYS with the Peng-Robinson algorithm. Turbines with designed inlet pressures of 25 MPa and 30 MPa and inlet temperatures ranging from 300°C to 600°C, as considered from previous studies, are used for impact analysis. Optimized shaft power ranging from 10 MW to 2,000 MW (one-flow configuration) is incorporated into the modeling to examine the effect on overall cycle efficiency. System efficiency is calculated, and key difficulties are highlighted to provide depth to the study. Turbines with synchronous revolutions (50 Hz) offer the highest efficiency for shaft power in one-flow configurations up to 500 MW, corresponding to a turbine efficiency of around 85%. This study is essential to evaluate the cycle's feasibility for achieving hundred-megawatt power levels from all critical aspects. The results will aid researchers in critically analyzing the cycle and taking steps toward practical implementation. Additionally, the study elaborates on the steps to design axial flow turbines and identifies key factors involved.

## References

[1] Jan Stepanek, Jan Syblik, Slavomir Entler. Axial sCO2 high-performance turbines parametric design, Energy Conversion and Management (Elsevier), 274 (2022).

[2] Salah, S. Design and analysis of supercritical carbon dioxide axial turbines (Unpublished Doctoral thesis, City, University of London).

[3] Tianrui Deng, Xionghui Li, Qiuwang Wang, Ting Ma. Dynamic modelling and transient characteristics of supercritical CO2 recompression Brayton cycle, Energy (Elsevier), 180(2019).

[4] Yuandong Zhang, Minjun Peng, Genglei Xia, Ge Wang, Cheng Zhou. Performance analysis of S-$CO_2$ recompression Brayton cycle based on turbomachinery detailed design. Nuclear engineering and technology (Elsevier), 52 (2020).

# Effects of nanofluid flow rate and thermal conductivity on the response ime of heat spreader integrated microchannel heat sink

**Ganesan Narendran[1], N Gnanasekaran[2], Arumuga Perumal D[2,*]**

[1]School of Interdisciplinary Design and Innovation (SIDI), Indian Institute of Information Technology, Design and Manufacturing, Kancheepuram 600127, India
[2] Department of Mechanical Engineering, National Institute of Technology Karnataka, Suruthkal, Mangaluru 575025, India
*Corresponding author: e-mail: perumal@nitk.edu.in

**Keywords**: integrated microchannel, heat spreader, graphene oxide, nanofluid, thermal response time

In any microchannel cooling device, the response time distinctively varies due to the heterogeneous integration of the source and the sink. With the advent of ultra-large-scale integration (ULSI) technology, many thousands of embedded circuits can be effectively integrated with better packaging [1, 2]. Due to the local temperature gradients which are referred to as hot spots and the maldistribution of the fluid flow in the microchannel, there is a considerable change in the response time which can be investigated using non-Fourier heat conduction. A single-phase model has been adopted for the numerical study of laminar forced convection heat transfer of the rectangular microchannel. Fig. 1 shows the schematic of the computational domain with boundary conditions [Fig.1]. An in-house rectangular microchannel with a heat spreader experimental setup is developed to investigate the thermo-hydrodynamics of the heat sink with GO-water nanofluid as the working fluid. The experimental results show that the heat wave propagation in the heat spreader is highly directional and influenced by the flow rate and thermal conductivity of the nanofluid. Results also indicate continuous migration of heat flux on the heat spreader is predominant near the vicinity of the outlet of the microchannel.

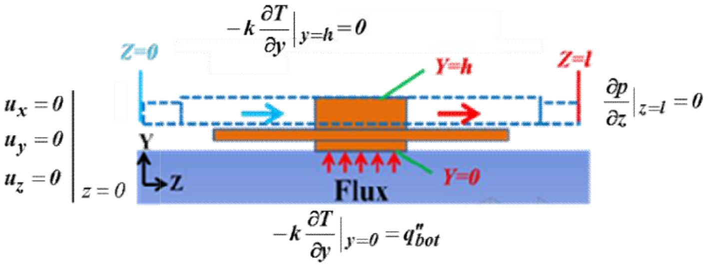


Fig. 1 : Schematic of the computational domain with boundary conditions

**References**
[1] G. Narendran, N. Gnanasekaran, D.A. Perumal, *Heat Transfer Engineering*, 41 (**2020**) 1252.
[2] G. Narendran, K. Ramachandran, N. Kumar, *Optik (Stuttg)*, 127 (**2016**) 817.

# Thermal characteristics of tubular energy storage system

**Pratyush Anand Burnwal [1], Pankaj Singh Manral [1], Ravi Kumar[1],**
**Anil Kumar Patil [1]*, Manoj Kumar [1]**

[1] Department of Mechanical Engineering, DIT University, Dehradun 248009, India
*Corresponding author: akpt1711978@gmail.com, dr.anilpatil@dituniversity.edu.in

**Keywords**: Thermal analysis, TESS, HTF.

Sensible energy storage system offers a reliable solution for thermal energy storage for a wide range of thermal applications. The thermal performance of storage system largely depends on temperature distribution in the storage matrix during charging/discharging process. Several materials and geometries of sensible energy storage have been investigated.

Cristofari et al. [1] found in a study that the temperature gradient in the solar thermal energy storage governs the thermal performance. Concrete has emerged as a material of choice because of its good mechanical strength, lower cost, and ability to withstand heat. Salomoni et al. [2] proposed the first concrete model of energy storage for solar power plants with the help of the Finite Element Method. Sujit and Biplab [3] optimized the concrete storage parameters to maximize heat transfer.

The present study explores the thermal characteristics of tubular energy storage system (TESS) at a mass flow rate of 0.018 kg/s for heat transfer fluid (HTF) by varying the HTF temperature from 45 to 85 °C.

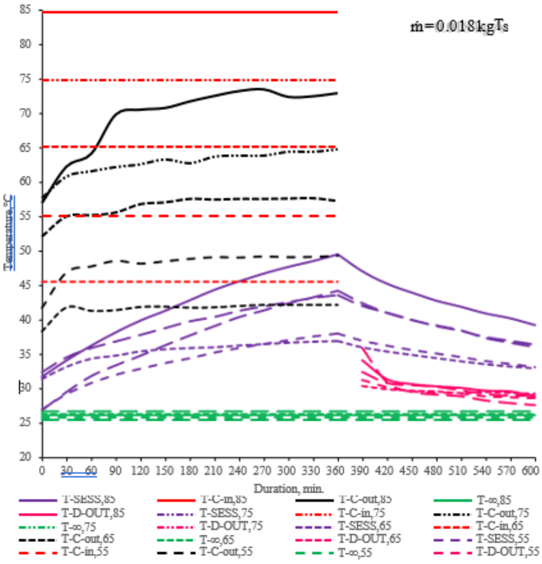


Fig. 1 : Temperature variation of TESS for charging/discharging cycle.

Figure 1 shows that the outlet HTF temperature has a significant rise during the charging period at higher HTF inlet temperatures. The temperature variation of TESS reveals that the thermal energy drains out completely from the system at lower HTF inlet temperature during the discharging period. For the same discharging time, the energy is still in the possession of storage system for further utilization.

## References

[1] Cristofari, C., Notton, G., Poggi, P., Louche, A., 2003. Influence of theflow rate and the tank stratification degree on the performances of a solar flat-plate collector. International Journal of Thermal Sciences 42,455–469.

[2] V.A. Salomoni, Carmelo E. Majorana, Giuseppe M. Giannuzzi, Adio Miliozzi, Rosa Di Maggio, Fabrizio Girardi, Domenico Mele, Marco Lucentini, "Thermal storage of sensible heat using concrete modules in solar power plants", Solar Energy,volume- 103,Pages: 303-315, 2014.

[3] Sujit R., Biplab K. D., "Heat transfer enhancement of sensible energy storage for low temperature

**T2- OP 01**

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Intrinsic Hydration Kinetics of Inorganic Salts: A Case of $Li_2SO_4$

**NOBUYOSHI KOGA[1]*, MITO HOTTA[1], LOIC FAVERGEON[2]**

[1] Grad. Sch. Humanities and Social Sciences, Hiroshima Univ., Higashi-Hiroshima 739-8524, Japan
[2] Mines Saint-Etienne, University of Lyon, Centre SPIN, Saint-Etienne, F-42023, France
*Corresponding author: e-mail: nkoga@hiroshima-u.ac.jp

**Keywords**: hydration, inorganic salts, humidity-controlled TG, water vapor pressure

The reversible thermal dehydration of inorganic hydrates can be promising candidate for designing thermochemical energy storage cycle comprising endothermic thermal dehydration and exothermic hydration of anhydride. Kinetics of the thermal dehydration of inorganic hydrates has been extensively studied last century, and the outcomes significantly contributed toward the establishment of the kinetic theory of the thermal decomposition of solids [1]. Besides, the hydration kinetics of inorganic salts is still on the way to establish the theoretical basis. In this study, phenomenology of the hydration of inorganic anhydride to form hydrated salts at various controlled temperatures ($T$) and water vapor pressures ($p(H_2O)$) was investigated using a humidity-controlled TG (HUM-TG, Rigaku), as exemplified by the hydration of $Li_2SO_4$ because the reverse reaction, i.e., the thermal dehydration of $Li_2SO_4 \cdot H_2O$, is one of the most studied reaction [2].

The hydration of $Li_2SO_4$ is the exothermic process:

$$Li_2SO_4(s) + H_2O(g) \rightarrow Li_2SO_4 \cdot H_2O(s) \qquad \Delta_r H^{\circ}_{298} = -57.0\ \mathrm{kJ} \qquad (1)$$

The reaction rate increases with increasing $p(H_2O)$ at a constant $T$ and with decreasing $T$ at a $p(H_2O)$. The kinetic behavior is universally described by the kinetic equation as a function of $T$, degree of reaction ($\alpha$), and $p(H_2O)$ as in the thermal dehydration at various $p(H_2O)$ values [2,3]:

$$\frac{d\alpha}{dt} = A\exp\left(-\frac{E_a}{RT}\right) f(\alpha)\, h\left(p(H_2O), P_{eq}(T)\right)$$

$$\text{with} \qquad h\left(p(H_2O), P_{eq}(T)\right) = p(H_2O)^{a}\left[1-\left(\frac{P_{eq}(T)}{p(H_2O)}\right)^{b}\right] \qquad (2)$$

where $A$, $E_a$, and $P_{eq}(T)$ are the Arrhenius preexponential factor, apparent activation energy, and equilibrium pressure of the reaction, respectively. By optimizing the exponent ($a$, $b$) in the accommodation function (AF; $h(p(H_2O), P_{eq}(T))$), the reaction rate ($d\alpha/dt$) at various $T$, $\alpha$, and $p(H_2O)$ can be described by Eq. (2). However, the apparent $E_a$ value determined based on Eq. (2) exhibits a negative value, because Eq. (2) describes the temperature dependences of $d\alpha/dt$ and $P_{eq}(T)$. The intrinsic $E_a$ value of the Arrhenius-type temperature dependence of $d\alpha/dt$ can be determined by subtracting the van't Hoff-type temperature dependence of $P_{eq}(T)$ from the results based on Eq. (2) [3]. The same can be done for determining the intrinsic $A$ value.

**References**

[1] N. Koga, H. Tanaka, *Thermochim. Acta*, 388 (**2002**) 41–61.
[2] Y. Yamamoto, L. Favergeon, N. Koga, *J. Phys. Chem. C*, 124 (**2020**) 11960–11976.
[3] M. Hotta, N. Koga, *Thermochim. Acta*, 733 (**2024**) 179699.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermal decomposition of polymer blends: A direct mathematical deconvolution of thermogravimetric curves

**TIBOR DUBAJ[1]*, STEFANO VECCHIO CIPRIOTI[2]**

[1] Institute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology,
Slovak University of Technology in Bratislava, Radlinskeho 9, SK-81237 Bratislava, Slovakia
[2] Department of Basic and Applied Science for Engineering, Sapienza University of Rome, Via del
Castro Laurenziano 7, Building RM017, I-00161 Rome, Italy.
*Corresponding author: e-mail: tibor.dubaj@stuba.sk

**Keywords**: Fraser—Suzuki function, decomposition kinetics, isoconversional method

For industrial processes, it is important to avoid degradation of materials by exceeding their processing time or temperature limits. Polymer blends are especially problematic as each component may unpredictably affect the blend stability. Here we report on kinetic analysis of thermal degradation of biodegradable polymer blends (PLA, PHBV, and PBAT) based on incremental isoconversional method [1] coupled with mathematical deconvolution of thermogravimetric (TG) curves. The measured kinetic envelope was decomposed into contributions approximately corresponding to degradation of each constituent of a blend. Kinetic parameters from isoconversional analysis were further used for estimating the effect of blending on thermal stability of constituents. Compared to the conventional approach, the deconvolution analysis was carried out directly on integral $\alpha(T)$ curves, thus bypassing the need to work with differential data $d\alpha/dt$ [2]. The TG curves were fitted by a weighed sum of Fraser—Suzuki functions in integral form:

$$\alpha(T) = \sum_{k=1}^{n} \frac{1}{a_{0k}} \int_{T_0}^{T} F(\mathbf{p}_k, T)\, dT,$$

where each mass-loss stage is described by a single Fraser—Suzuki term

$$F(\mathbf{p}_k, T) = a_{1k} \exp\left\{ -\frac{\ln 2}{a_{4k}^2} \left[ \ln\left( 1 + 2a_{4k} \frac{T - a_{2k}}{a_{3k}} \right) \right]^2 \right\}.$$

Subsequent isoconversional kinetic analysis of deconvoluted $\alpha_k(T)$ curves allows to calculate various parameters for assessing the effect of blending on thermal degradation, for example, by comparing the decomposition half-time $t_{1/2}$. The results can be made robust by using relative criterion such as $t_{1/2}$(blend)/$t_{1/2}$(neat polymer).

**Acknowledgement**
Financial support from the Slovak Scientific Grant Agency (VEGA 1/0498/22) is acknowledged.

**References**

[1] T. Dubaj, Z. Cibulková, P. Šimon, *Journal of Computational Chemistry* 36 (**2015**) 392
[2] T. Dubaj, S. Vecchio Ciprioti, J. Tirillò, F. Sarasini, *Thermochimica Acta* 736 (**2024**) 179761.

# Mixed Alkali Effect on Crystallization Kinetics of Lithium Metaphosphate Based Solid Electrolyte Glassy Systems

**BENSON K. MONEY[1]*, K. HARIHARAN[2]**

[1]Department of Sciences and Humanities, School of Engineering & Technology,
Christ (deemed to be University), Bangalore-560074, India
[2]Formerly Professor of Physics, Indian Institute of Technology Madras, Chennai-600036, India
*Corresponding author: e-mail: benson.money@christuniversity.in

**Keywords**: Superionic conducting glass, DSC, Mixed Alkali Effect

The ionic conductivity of mol% 50Li2O–50P2O5 melt quenched glass shows an anomalous increase after its glass transition temperature around 590 K. On further increasing the temperature gradually, the conductivity decreases owing to the devitrification of Li2O–P2O5 glass [Fig. 1]. The evolution of devitrified crystallites was evidenced by XRD patterns. The DSC studies showed that the crystallization mechanism is closely associated with the JMA.

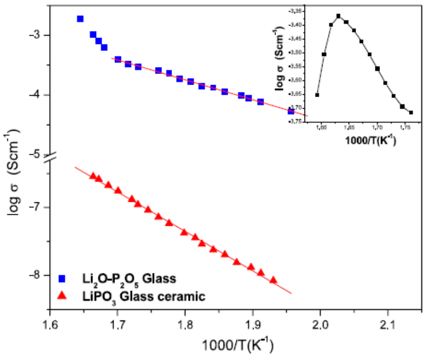


Fig1. Arrhenius plot

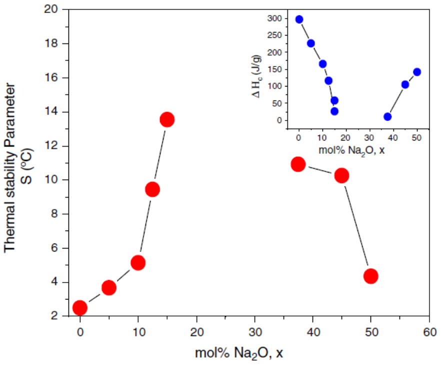


Fig2. Thermal parameters

The effect of second glass modifier Na2O on the crystallization kinetics and thermal stability of the mol% xNa2O:(50−x)Li2O:50P2O5 glasses is also investigated. The DSC studies showed the classical 'mixed alkali effect' on the glass transition temperature, with the Tg minima for the glass composition, x=25mol%. The presence of small concentration of second alkali tends to thermally stabilize the intermediate compositions of mol% xNa2O:(50−x)Li2O:50P2O5 as these compositions exhibited high thermal stability parameter, high activation energy for crystallization and low enthalpy of crystallization [Fig. 2].

## References

[1] St Adams, K. Hariharan and J. Maier, *Solid State Phenom.* 39/40 **(1994)** 285.
[2] H. Yinnon and D. R. Uhlmann, *J. Non-Cryst. Solids* 54 **(1983)** 253.
[3] D.E. Day, *J. Non-Cryst. Solids* 21 **(1976)** 343–372.
[4] B.K. Money, K. Hariharan, *J. Phys. Condens. Matter* 21 **(2009)** 115102.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Pyrolysis Of Sesame Stalk Using Non-Isothermal Thermogravimetric Analysis: Thermo-Kinetic Studies Using Model-Fitting And Model-Free Method

**ANUSHA GURURAJAN AND CHITHRA K***

Nanomaterials and Environmental Research Laboratory, Department of Chemical Engineering,
Alagappa College of Technology, Anna University, Chennai, Tamil Nadu, India – 600025
*Corresponding author: chitrakumaran@yahoo.co.in

**Keywords:** Sesame stalk, thermogravimetric analyses, kinetic triplets, model-free, model-fitting, master plots.

The kinetic triplets data is essential for designing pyrolysis reactor. Present work aimed to investigate the pyrolysis kinetics of waste sesame stalks (SS). The novelty of this work is the evaluation of kinetic triplets using model-fitting and model-free combined with Criado's z(α) master plots methods. The thermogravimetric analyses were performed on SS from 28 – 900 °C at three heating rates 10, 20 and 30 °C/min. The average activation energy using Kissinger-Akahira-Sunose, Flynn-Wall-Ozawa and Starink methods were 144.04, 146.28 and 143.93 kJ/mol respectively. The preexponential factors were obtained for models found using master plots. The modelfitting Coats-Redfern method was performed for 21 different reaction models. 1.5$^{th}$, 2$^{nd}$ and 3$^{rd}$ order of R was found to the best fit in master plot and CR method. The kinetic data obtained are reliable as the linear regression values ($R^2$) for the plot were > 0.99 and 0.91 for model-free and model-fitting methods respectively.

**References**

[1] S. Vyazovkin *et al.*, *Elsevier B.V.* (**2020**)

[2] M. E. Brown *et al.*, "Computational aspects of kinetic analysis Part A: The ICTAC kinetics projectdata, methods and results $."

[3] M. Raza, B. Abu-Jdayil, A. H. Al-Marzouqi, and A. Inayat, *Renew Energy*, 183 (**2022**) 67–77.

[4] A. Tagade, S. Kandpal, and A. N. Sawarkar, *Bioresour Technol*, 391 (**2024**)

`

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# A predictive multiple-distribution DAEM modeling of the impact of embedded salts on bitumen thermal behavior

**ALI HODROJ**[1,2,*], **NICOLAS COURTOIS**[1], **SIMON DELCOUR**[3], **DAMIEN MARQUIS**[3], **CHARLES BRISSOT**[1], **PATRICK PERRE**[2]

[1]CEA, DES, ISEC, DPME, Univ. Montpellier, Marcoule, France
[2]Université Paris-Saclay, CentraleSupelec, LGPM, 91190 Gif-sur-Yvette, France
[3]LNE (National Laboratory for Testing and Metrology), 78197 Trappes Cedex, France
*Corresponding author: e-mail: ali.hodroj@cea.fr

**Keywords**: bituminized waste products, DAEM, kinetic modeling, mass loss, TGA

During the 60s, bitumen was chosen by the French nuclear industry as a matrix for encapsulating low and intermediate-level wastes generated during nuclear fuel reprocessing. In order to ensure safe storage and disposal regarding fire hazard, the thermal reactivity of the bituminized wastes should be investigated. The primary focus was to comprehensively understand the thermolysis processes using Thermogravimetry resulting from a simplified system (pure bitumen) [1]. Then, complexity augmentation entails the inclusion of salts ($NaNO_3$, $Mg[NO_3]_2 \cdot xH_2O$) commonly found in bituminized wastes. To capture the intricate details of the reactions involved in bitumen–salts mixes, a multi-Distributed Activation Energy Model (DAEM) [2] is proposed. Isothermal and dynamic thermogravimetric experiments were conducted for data identification and validation, respectively. The model demonstrates valuable applicability, signifying its reliability and robustness in determining and predicting kinetics across a broad spectrum of temperatures and durations. The 2-Gaussians distribution yields a strong predictive performance of pure bitumen thermolysis under nitrogen (Figure *1*). However, modeling of the thermal behavior of bitumen-salts mixes will requires the utilization of more sophisticated distributions, including non-symmetrical functions [3].

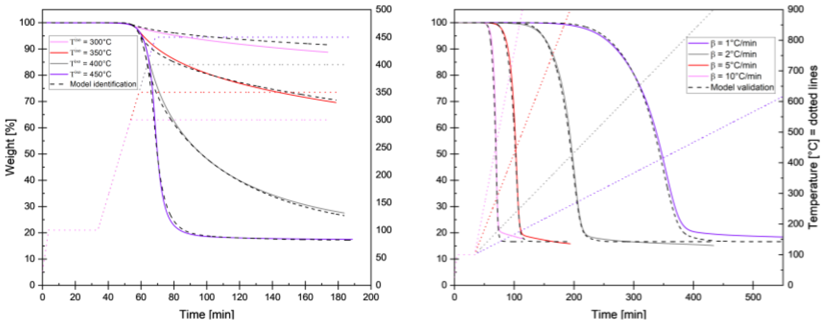


Figure 1, 2-Gaussian DAEM identification (left) and validation (right) of pure bitumen under $N_2$

**References**

[1] G. Matta et al., Thermochim. Acta, vol. 724, p. 179514, Jun. 2023.
[2] V. Vand, Proc. Phys. Soc., vol. 55, no. 3, p. 222, May 1943.
[3] P. Perré et al., Fuel, vol. 288, p. 119692, Mar. 2021.

**T2- OP 06**

# Development of a $TiO_2$ Nanoparticle Coating-Based Plasma Torch for Eco-Friendly Disposal of Municipal Solid Waste

**SHUBHRO CHAKRABARTTY [1], PRADIP KUMAR CHATTERJEE[2*]**

[1]Assistant Professor (D.Y. Patil International University
Akurdi, Maharashtra, India)
[1]Department of Computer Science Engineering and Applications, DYPIU, Akurdi, India
[2]CSIR Central Mechanical Engineering Research Institute, Durgapur – 713209, India
Corresponding author: e-mail: pradipcmeri@gmail.com

**Keywords**: Nanoparticles, thermal analysis, waste to energy, citrate precursor, optical properties

The continuous accumulation of Municipal Solid Waste (MSW) without proper disposal methods has become a significant manmade issue that demands immediate action and careful precautions. Allowing MSW to decay naturally releases large amounts of methane, which worsens global warming. Additionally, the toxins generated from MSW pose serious health risks, including fatal diseases like cancer. Fortunately, plasma technology offers a viable solution for waste disposal, providing a safe and toxin-free process that can be effectively implemented. Plasma technology has been successfully used for various types of waste, eliminating the need for segregation. Efforts are currently underway to extract usable energy from this process. The efficiency of plasma-based disposal systems depends greatly on the performance of the plasma torch. Several factors influence the plasma torch's effectiveness, including electrode material erosion, the gap between electrodes, the carrier gas and its flow rate, electrode cooling, and the power supply's voltage and frequency. To improve torch efficiency, it's crucial to generate plasma mass and maximize energy content. To address electrode erosion and enhance surface roughness, a $TiO_2$ nanoparticle (NPs) coating is employed. This coating helps improve the durability and efficiency of the plasma torch, which is crucial for generating plasma mass and maximizing energy content. Efficient operation involves maximizing energy from electron discharge and delivering it effectively to the target, ensuring the system's optimal performance.

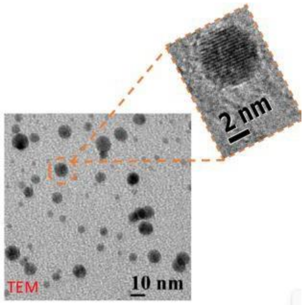


Figure 1: The TEM image of grown $TiO_2$ NPs

## References

[1] N. Venkat Ramani, Current Science, vol. 83, no. 3, 2002.
[2] R. Joshi and S. Ahmed, Cogent Environmental Science, vol. 2, article 1139434, 2016.
[3] CPCB (Central Pollution Control Board), 2016.
[4] M. Sharholy, A. Khafeel, M. Gauhar, and R. C. Trivedi, Journal, vol. 28, no. 2, pp. 459-467, 2007.
[5] S. Chakrabartty, S. Kumar, H. Song, and M. Jeon, Journal of Nanoscience and Nanotechnology, vol. 18, pp. 1-5, 2018.

# Pyrolysis of waste printed circuit board: kinetic analysis and detail product characterization

**BIBARI BORO*, PANKAJ TIWARI**

Department of Chemical Engineering, Indian Institute of Technology Guwahati, Assam-781039, India
*Corresponding author e-mail: b.bibari@iitg.ac.in

**Keywords**: Waste printed circuit board, Thermal gravimetric analysis, Kinetic triplets, Isoconversional models, Gas chromatography.

The waste printed circuit board (WPCB) is a valuable component of E-Waste stream because of the presence of valuable metals and it is also considered hazardous due to the presence of harmful chemicals and heavy metals [1]. Hence, developing a proper recycling process for the WPCB is essential from the economic as well as environmental point-of-view. In the current study, pyrolysis was proposed as a recycling process for WPCB. WPCB from computer system (motherboard) were procured and the electronic components were dismantled followed by cutting into 1 cm × 1 cm size chips. The WPCB was characterized using proximate, ultimate, FTIR and TG-DTG analyses. The TG-DTG analysis was performed at heating rates of 5, 10, 20 and 50 ℃/min from 30 to 1000 ℃ to obtain the kinetic parameters. The organic degradation range was found to be in the range of 250 – 450 ℃ depending on the heating rate program. The average activation energies were found to be 143.7, 146.3, 135.6 and 136 kJ/mol, for the Friedman, FWO, KAS and Starink, respectively. The Criado master plot analysis showed that the thermal degradation followed F1 model and the pre-exponential factor were found to be in the range of $6.50\times10^{8}$ – $2.03\times10^{10}$ 1/s [2]. The conversion profile (activation energy vs conversion) was further reconstructed using MATLAB software to validate the kinetic parameters. Starink method showed highest similarity with $R^2$ value of 0.9946. The WPCB was pyrolyzed at 500 ℃, 10 ℃/min and hold-time of 60 min in a semi-batch system, fixed bed reactor using $N_2$ gas to create the inert environment. The liquid fraction was characterized using FTIR, NMR ($^1$H and $^{13}$C) and GC-MS which showed presence of high aromatic content, mainly phenolic compounds. The physical characteristics such as density and calorific values were found to be 1.07 g/cm$^3$ and 34 MJ/kg, respectively. The gas fraction was analysed for its composition using GC-FID and GC-TCD. The analysis showed the presence of $H_2$ (25 vol%), majorly and minor concentrations of $CH_4$, CO, $CO_2$ and $C_1$-$C_4$ hydrocarbon gases. The char produced was characterized and compared with raw WPCB for the effect of thermal degradation characteristics using FTIR, ultimate analysis and FESEM.

## References

[1] D.R Tipre, B. R. Khatri, S. C. Thacker and S. R. Dave, *Environmental Science and Pollution Research*, 28 (**2021**) 10503-10518.
[2] B. Boro and P. Tiwari, *Thermochimica Acta*, 736 (**2024**) 179747.

# Study of σ → α phase transformation kinetics of Fe-48.5 at.% V alloy by using DSC

**DASARATH MAJI[1*], BISWAJIT SAMANTA[1], S. BALAKRISHNAN[1]**

[1]MC & MFCG, Indira Gandhi Centre for Atomic Research, Kalpakkam 603102, India
*Corresponding author: e-mail: dmaji@igcar.gov.in

**Keywords**: Phase transformation; Kinetics; Activation energy; DSC

Vanadium-based alloys have great interest as protective coatings in sodium and lithium-cooled nuclear reactors [1] due to its less fragile to neutronic radiation and have the best mechanical characteristics at high temperatures. This paper reports the findings of an experimental investigation of σ → α phase transformation kinetics by using DSC. Arc-melting was used to prepare the Fe-48.5 at.% V alloy. The alloy was annealed at 1073 K for 72 h to obtain the σ phase. For the synthesis of the α phase, the as-casted alloy was water quenched from 1523 K to 273 K. Rietveld refinement of X-ray powder diffraction data was used to ascertain its crystal structure and lattice parameter. The typical XRD pattern for the σ phase is shown in Fig. 1 (a). To investigate the kinetics of σ → α phase transformation, the alloy was heated at different heating rates (from 2 K min$^{-1}$ to 50 K min$^{-1}$) by using a high-temperature heat flux DSC. A prominent thermal arrest was observed around 1420 K and its variation with heating rate is shown in Fig. 1(b).

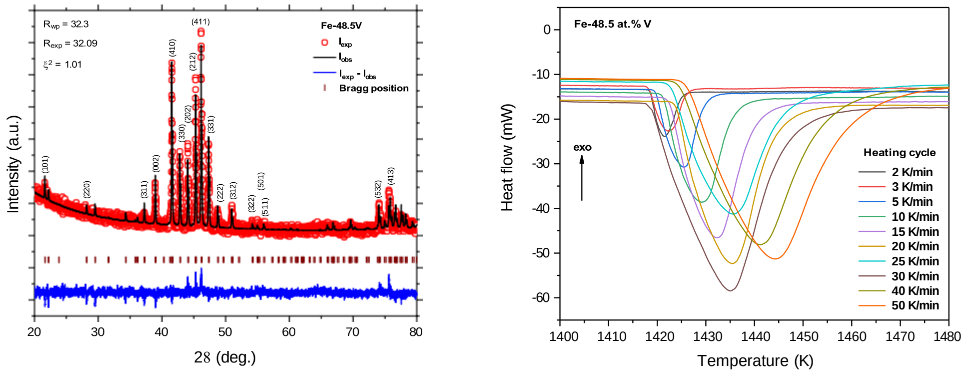


**Fig. 1 (a)** Rietveld refinement of the XRD pattern for annealed Fe-48.5 at.% V alloy; **(b)** DSC of Fe-48.5 at.% V recorded at different heating rate from 2 to 50 K/min

Phase transformation kinetics were analysed by employing Kissinger and Ozawa method [2]. The activation energy was found to be 2117 and 2140 kJ mol$^{-1}$, respectively. These values are reported for the first time. It is evident that, the activation energy found in both the methods was comparable to each other.

**References**

[1] R. Teghil, L. D'Alessio, V. Marotta, A. Santagata, G. De Maria, D. Ferro, M.A. Sanson, Applied surface science 119 (1997) 34-40.

[2] T. Ozawa, J. Therm. Anal. 2 (1970) 301–324.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# MOF-derived Perovskite Oxide SrTi1-xCoXO3-δ as Anion-intercalated Electrode Material for Supercapacitor

**GEETA CHAUDHARY, PROF RAJ KISHORE SHARMA***

Department of Chemistry, University of Delhi, 110007 India *Corresponding author: e-mail: rajksharma@chemistry.du.ac.in

**Keywords**: MOF derived perovskites; SrTi1-xCoxO3-δ; Anion intercalation; Oxygen vacancies; Supercapacitor

Herein, we have employed a MOF derived approach to synthesize SrTi1-xCoxO3-δ (STO-Co) at various doping ratios (x = 0, 0.5, 1, 2, and 3 %) for anion-intercalated supercapacitor electrode. The synthesis strategy resulted into a quick and room temperature synthesis of the materials. Morphological alterations were also observed in the native SrTiO3-δ (STO) as the dopant's concentration varied from 0 to 3%. Elongated needle-like morphology of STO-Co-2% induced an exceptionally high electrochemically active surface area (ECSA) of 2388 m2 g-1. Cobalt doping also lowered the band gap of STO from 3.4 eV to 2.7 eV in STO-Co-2%, implying rich electronic conductivity of STO-Co-2% electrode. Enhancement in oxygen vacancies was also observed which further boosted the anion-intercalated energy storage. This altogether attributed towards the highest specific capacitance of 1311 F g−1 @ 2 A g−1 for STO-Co-2%. Fabricated STCO||STCO symmetric cell resulted in an energy density of 38 Wh Kg-1 @575 W Kg-1 with a working voltage of 1.2 V and outstanding cycling stability with 94.7% retention after 5000 GCD cycles @ 5 A g1.

**T2- OP 10**

# Thermal and Catalytic Liquefaction of Northeastern Indian Coals with Tetralin and Toluene: Kinetic Modelling, Mechanisms and Product Characterization

**Govind Dubey[1], Prabu vairakannu[1], Pankaj Tiwari[1*]**

[1]Department of Chemical Engineering, Indian Institute of Technology Guwahati, Assam-781039, India
*Corresponding author: e-mail: pankaj.tiwari@iitg.ac.in

**Keywords**: Direct coal liquefaction, Catalyst, Kinetic modelling, Reaction mechanism

With the ongoing increase in energy needs, countries, especially developing ones, are continuously searching for indigenous energy sources to achieve self-reliance in energy. At present, India heavily depends on coal to meet its energy requirements [1]. Although coal is found throughout India, much of it is of low-grade [2]. One effective method of upgrading is direct coal liquefaction (DCL) process. To study the effect of temperature, catalyst, and residence time on the direct coal liquefaction (DCL) we carried out the experiments with iron-based catalyst ($Fe_2O_3$) in a 200 ml stainless steel high-pressure reactor. The present study examined three northeastern Indian coals (high, medium, and low ash) within a temperature range of 400-450°C, using tetralin and toluene as solvents. The two solvents used have different hydrogen donation properties: tetralin is an $H_2$ donor, while toluene is non-$H_2$ donor. A kinetic model was proposed, using which the kinetic parameters were estimated. The obtained model values were further used to reconstruct the concentration profiles of products and compared with the experimental values. The process yielded gaseous, liquid, and solid products, along with water. The liquid products were further divided into three types based on their solubility: oil (hexane soluble), asphaltene (toluene soluble), and preasphaltene (tetrahydrofuran soluble). The AB coal was found to have the highest oil yield of 42.33wt% and 16.25wt% at 450°C with 1 hr residence time and 1 wt% of catalyst for tetralin and toluene respectively. The activation energy was reduced with the use of the catalyst, which resulted in an increased yield of products, especially gas and oil. These products were analyzed using GC-TCD/FID/PFPD, FTIR, $^1H$ NMR, HRMS, and FESEM. The results showed that the $H_2$ transfer mechanism was dominant for tetralin, while the $H_2$ shuttling mechanism was dominant for toluene. The present study helps to develop understanding of DCL for Indian coals with different solvents.

## References

[1.] Dong, L., H. Vuthaluru, D. French, S. Karmakar, A.K. Sutrakar, and R. Satyakam, Indian coal pyrolysis behaviour and kinetics study using covalent bond information. Thermochimica Acta, 711 (2022).

[2.] Kumar, R., V. Bansal, R.M. Badhe, I.S.S. Madhira, V. Sugumaran, S. Ahmed, J. Christopher, M.B. Patel, and B. Basu, Characterization of Indian origin oil shale using advanced analytical techniques. Fuel, 113 (2013).610-616.

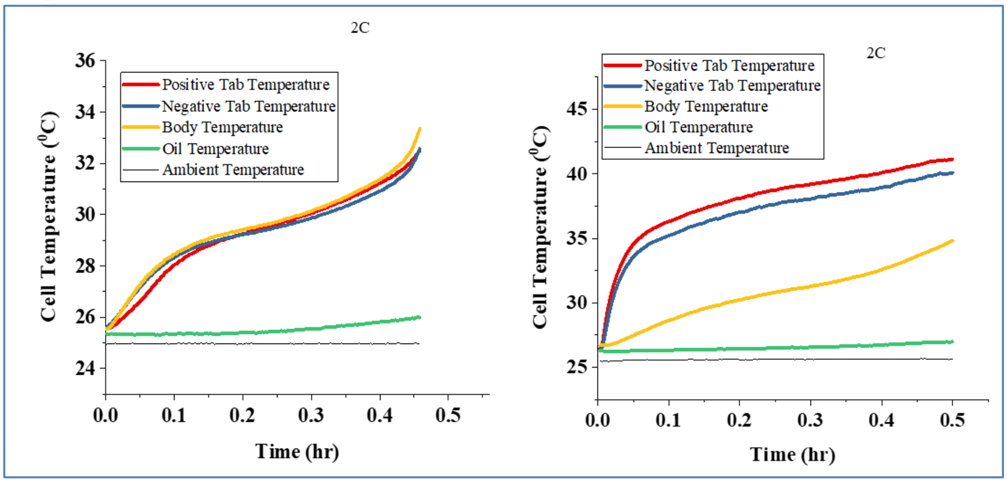
# Evaluation of Cooling Effectiveness for Cylindrical and Prismatic Batteries Using Oil Immersion Cooling System

**HEMAVATHI S[1]*, THIRU KUMARAN A[1]**

[1] CSIR - Central Electrochemical Research Institute-Madras Unit, CSIR Madras Complex, Taramani, Chennai - 600 113, India
*Corresponding author: e-mail: hemavathi@cecri.res.in

**Keywords**: thermal analysis, Li-ion battery, immersion cooling

This study evaluates the thermal performance of cylindrical and prismatic lithium-ion cells under natural air cooling and oil immersion cooling conditions. The experiment is conducted at 25 °C with a 2C discharge rate, the cylindrical cells (NMC chemistry, 3.6V, 2.5Ah) and prismatic cells (LFP chemistry, 3.2V, 40Ah) demonstrated significant differences in thermal management. Under natural air cooling, cylindrical cells had a body temperature of 41.5 °C with the negative and positive tabs at 40.1 °C and 34.5 °C, respectively, while prismatic cells showed a body temperature of 39.3 °C and higher tab temperatures of 45.5 °C and 44.2 °C. In contrast, oil immersion cooling achieved lower and more uniform temperatures, with cylindrical cells reaching a body temperature of 32.4 °C and tabs at 31.8 °C and 32.0 °C, and prismatic cells at 34.8 °C with tabs at 40.1 °C and 41.1 °C. This study highlights the superior thermal management of oil immersion cooling, particularly for cylindrical cells, and underscores the challenges in achieving uniform cooling for prismatic cells.



(a) (b)

Fig. 1 : Thermal distribution of oil-immersion cooled (a) Cylindrical cell (b) Prismatic cell, at 2C rate

## References

[1] S. Hemavathi, Srirama Srinivas, A.S. Prakash, *Journal of Energy Storage*, Vol. 72, D, 2023.

# Pyrolysis of petroleum pitch: Thermogravimetric analysis and non-isothermal kinetics using the distributed activation energy model (DAEM)

**Khokan Sahoo**[1*], **Kanuparthy Naga Raja**[2], **Neeraj Kumbhakarna**[3], **Sudarshan Kumar**[1]

[1]Department of Aerospace Engineering, Indian Institute of Technology Bombay, Powai-400076, Mumbai

[2]Hindustan Petroleum Corporation Limited, Corporate Green Research and Development Centre, Bengaluru-560067

[3]Department of Mechanical Engineering, Indian Institute of Technology Bombay, Powai-400076, Mumbai

[*]Corresponding author mail id: khokanwellcome@gmail.com

**Keywords**: thermal analysis, TGA, DTA, kinetics, activation energy

The pyrolysis characteristics of petroleum pitch were investigated using the thermogravimetric analysis (TGA) to develop a mechanistic understanding of the complicated decomposition process kinetically and thermodynamically. The single-step weight loss was observed at all the heating rates with peak weight loss temperatures of 446, 462, 469, and 481 °C at 2.5, 5, 10, and 15 °C/min. The distributed activation energy model [1] successfully captured the pyrolysis kinetics, and the variation of activation energy was observed. The activation energy varied from 85.94 to 193.39 kJ/mol in the conversion range of 0.1-0.9, with an average of 152.22 kJ/mol. The thermal characteristics and kinetics parameters are presented in Fig. 1 and Fig. 2. The variation of activation energy and thermodynamic parameters confirmed the complicated nature of the pitch pyrolysis process and the influence of complex compositions like aromatic hydrocarbon and heteroatoms.

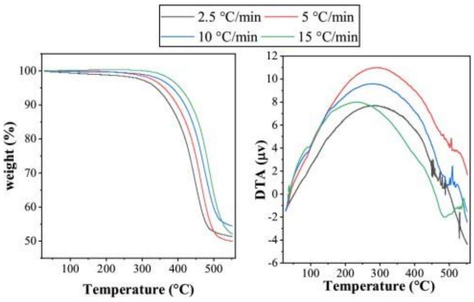


Fig. 1: Thermal characteristics Curve

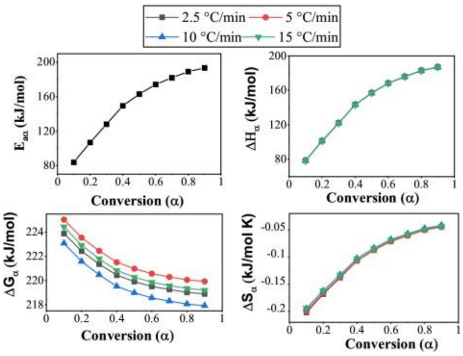


Fig. 2: Kinetics parameters

## References

[1] Fan C, Zan C, Zhang Q, Ma D, Chu Y, Jiang H, Shi L, Wei F. The oxidation of heavy oil: Thermogravimetric analysis and non-isothermal kinetics using the distributed activation energy model. Fuel processing technology. 2014 Mar 1;119:146-50.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Co-combustion of Biochars: Thermogravimetric Analysis and Distributed Activation Energy Modeling

**PRITAM KUMAR, PIYUSH CHAUNSALI AND RAVIKRISHNAN VINU***

Chemical Engineering Department, Indian Institute of Technology Madras, India, 600036
Civil Engineering Department, Indian Institute of Technology Madras, India, 600036
*Corresponding author: e-mail: vinu@smail.iitm.ac.in

**Keywords**: Co-combustion, lignocellulosic biomass, biochar, distributed activation energy modeling

This study explores the combustion characteristics and kinetic of biochars (bagasse char, rice straw char and rice husk char) and biochar binary blends, and findings were compared with coal and parent biomasses. All materials were characterized using proximate, ultimate, higher heating value and Fourier transform infrared spectroscopy analyses. Combustion experiments were performed using the thermogravimetric analysis. Various combustion characteristics parameters, such as ignition temperature, peak temperature, burnout temperature and maximum combustion rate, were evaluated to know the combustion performance of different samples. Results signified that combustion process of biochars is great extent similar to coal. The combustion kinetic of coal, biomasses, biochars and biochar binary mixtures was simulated with distributed activated energy modeling. Biochars and biochar blends combustion was described using two pseudo components, viz., lignin and char, and biomass using three pseudo components, hemicellulose, cellulose and lignin. Whereas, coal combustion was derived with two pseudo components, such as volatile matter and fixed carbon. For biochar combustion, out of two pseudo components, activation energy was found to be highest for char (247.6 kJ/mol) and lowest for lignin pseudo component. Among different biochars, activation energy varied exclusively for lignin combustion. For lignin combustion, activation energy was maximum for bagasse char (175.5 kJ/mol) and minimum for rice straw char (130.8 kJ/mol). Combustion of biochar blends follows a straightforward binary mixture rule, with no synergistic mechanisms present. Fuel consumption, ash generation, heat release rate and burning time analysis signify that coal can be replaced with biochars and their binary blends.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermal Impact of PCM Thickness on a Cylindrical Li-ion Cell

**PRITAM BHAT[1], MAHESH K. VARPE[2]***

[1]Department of Mechanical and Manufacturing Engineering,
[2] Department of Automotive and Aeronautical Engineering,
M. S. Ramaiah University of Applied Sciences, Bengaluru – 560058, India
*Corresponding author: e-mail: maheshvarpe@gmail.com

**Keywords**: PCM, battery thermal management, Li-ion battery, heat generation

Electric vehicles (EVs) preferably use lithium-ion (Li-ion) cells owing to their high energy density and low self-discharge rates. High power demand by the load, however, causes li-ion cells to discharge at higher C-rates, resulting in significant heat production and excessive cell temperatures. Therefore, battery thermal management (BTM) is necessary to effectively dissipate the excess heat generation by the cell at higher C-rates and contain the cell temperatures within the safe operating temperature range of 35°–50°C [1]. A passive thermal management substance such as PCM (phase change material) can absorb large amount of heat and minimizes temperature non-uniformity across the cell surface [3].

A Samsung INR18650-25R cylindrical cell with a voltage of 3.6 V and a capacity of 2.5 Ah is chosen as a baseline case. A multi-scale multi-dimension (MSMD) battery model with NTGK electrochemistry is considered for numerical analysis. The ambient temperature is at 35 °C. The validation of prediction from the numerical investigation with the experimental data [2] is found satisfactory. The current investigation uses RT-42 paraffin, a PCM, with the baseline case. A C-rate of 8C is considered to analyse the thermal behaviour of cell with PCM.

It is desired for the PCM to completely liquify ($\beta = 1$) before the end of cell discharge to effectively absorb the heat generated by the cell, in the form of its latent energy. It is observed that the cell temperature decreases significantly for PCM radial thickness greater than 0.25R ('R' is radius of cell) and remains almost invariant thereafter at ~ 50 °C. The liquid fraction ($\beta$) of the PCM is found to be nearly 1 for thickness up to 0.25R. The liquid fraction decreases considerably at the end of discharge with an increase in PCM thickness resulting in an increased cell temperature which is undesirable. Thus, an optimum thickness of the PCM in BTM not only increases the heat dissipation from the cell but also reduces the battery pack size and the weight by avoiding excessive PCM volume. Therefore, it is observed that 0.25*R is an optimal thickness to maintain the cylindrical cell temperature within a safe operating range.

## References

[1] Ma, Shuai, et al. "Temperature effect and thermal impact in lithium-ion batteries: A review." Progress in Natural Science, vol. 28, no. 6, Dec. 2018, pp. 653–66.

[2] SAMSUNG SDI, "Introduction of INR18650-25R.," datasheet, Oct. 2013.

[3] Wazeer, Adil, et al. "Phase change materials for battery thermal management of electric and hybrid vehicles: A review." Energy Nexus, vol. 7, Sept. 2022, p. 100131.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Numerical investigation of the effect of thermal energy storage materials on the performance of solar updraft tower (SUT) integrated with natural and forced draught systems

RAMAKRISHNA BALIJEPALLI[1]*, VALAPARLA RANJITH KUMAR[2], B.A.G. YUVARAJU[3]

[1]Department of Mechanical Engineering, Vignan's Lara Institute of Technology and Science, JNTUK Kakinada-522213, India
[2] Department of Mechanical Engineering, Vignan's Institute of Information Technology, Vizag-530049, India
[3]School of Mechanical Engineering, SASTRA Deemed to be University, Thanjavur-613401, India
Corresponding author: e-mail: bondaatchutaganesh@mech.sastra.edu

**Keywords**: thermal analysis, energy storage materials, solar updraft tower, natural draught, forced draught

Investigating the effect of thermal energy storage (TES) materials on the performance of a solar updraft tower (SUT) integrated with natural and forced draught systems is essential to enhance energy efficiency, optimize performance, and reduce costs. This paper aims to present two novel 3D numerical models for SUTs to enhance energy efficiency. Numerical simulations were performed on them to investigate the effect of TES materials on the performance of SUT integrated with natural and forced draught systems with different radiation intensities. Flow and fluid parameters such as pressure, velocity, and temperature were estimated and analyzed for two models such as model A (without TES system) and model B (with TES system), in two cases such as case I (natural convection) and case II (forced convection). Numerical simulations were performed in ANSYS 16 under steady-state conditions for model A with different constant global radiation values ranging from 750 W/m$^2$ to 1150 W/m$^2$. The simulations were performed for model A with case I and case II with inlet velocities ranging from 1 m/s to 3 m/s with an interval of 0.5 m/s with a constant radiation of 1150 W/m$^2$ to analyze the effect of the forced draught system in SUT. In addition, simulations for model B with different materials were performed by integrating the forced draught system.

The performance parameters such as velocity, pressure, and temperature gradually increased with the increase of the radiation intensity. At a radiation intensity of 750 W/m$^2$, the absorber plate temperature was 328 K, rising to 355 K at 1150 W/m$^2$. Correspondingly, the air velocity increased from 2.3 m/s to 2.89 m/s. The forced draught system creates positive pressure in the SUT, affecting its performance. The maximum velocity of air in SUT with inlet of 1 m/s was 5.07 m/s, which increases than natural convection, with inlet velocity of 3 m/s will raise the maximum velocity to 14.49 m/s. The simulation results showed the temperature of the absorber plate in case II of TES materials such as quartz, sandy gravel, loam, and sand & rock as 345 K, 346 K, 349 K, and 350 K, respectively.

# Revealing the Augmentation of Surface Immobilization of Adsorbed Nickel Chalcogenate during Alkaline Water Oxidation

**RISHABH MISHRA[1], MANISHA MALVIYA[1*]**

[1]Indian Institute of Technology, (BHU), Varanasi-221005
*Corresponding author: e-mail: manisha.apc@itbhu.ac.in

**Keywords**: Operando spectroscopy, Transition metals, Selenides, Electrocatalyst

Transition metal chalcogenides, composed of transition metals and chalcogens, have demonstrated significant effectiveness as pre-electrocatalysts for the oxygen evolution reaction (OER). Upon reaching OER conditions, these compounds undergo a transformation to metal (oxy) hydroxides. Nonetheless, the specific role of chalcogen in these materials post-oxidation and extensive leaching remains incompletely understood. Thus, the current research seeks to elucidate the crucial function of surface-adsorbed chalcogenides in enhancing the OER performance of these substances. To explore this occurrence, our focus is specifically on $NiSe_2$. Utilizing in situ operando UV-Vis spectroscopy, we observed the oxidation of Se-Se bonds, resulting in the creation of selenites ($SeO_3^{-2}$) and subsequently selenates ($SeO_4^{-2}$).

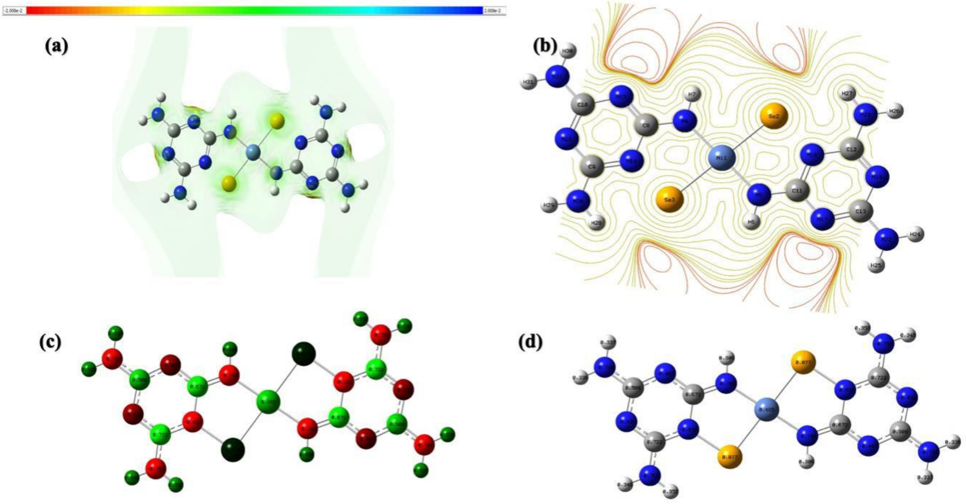


**Fig. 1** MEP of $NiSe_2$/C; **(b)**Contour line diagram of the electron density distribution of $NiSe_2$/C; **(c, d)** Mulliken atomic charges of $NiSe_2$@C complex.

**References**

[1] D. Taherinia, H. Hatami, F. M. Valadi, E. Akbarzadeh, *Energy & Fuels*, *36*(23), 14331-14340 (2022).

[2] I. H. Kwak, H. S. Im, D. M. Jang, Y. W. Kim, K. Park, Y. R. Lim, J. Park (2016), *ACS applied materials & interfaces*, *8*(8), 5327-5334.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Revolutionizing Sodium-ion Batteries: Efficient Ion Diffusion Analysis and State of Charge Prediction with Time Series Analysis

**SHIVARANJINI S[1]*, NEETU SRIVASTAVA[2]**

[1, 2] Department of Mathematics, Amrita School of Engineering, Amrita Vishwa Vidyapeetham,
Bengaluru, Karnataka, India
*Corresponding author: e-mail: s_neetu@blr.amrita.edu

**Keywords**: Batteries, Mathematical Modelling, State of charge, long short-term memory networks.

Sodium-ion batteries represent a significant advancement in energy storage technology due to their cost-effectiveness and the abundant availability of sodium. To enhance the modelling of these batteries, the problem of mass transport in electrode particles is considered in this paper which is based on Fick's second law and is represented as a partial differential equation (PDE). The modelled PDE is transformed into a dimensionless form by applying appropriate dimensionless variables. The obtained non-dimensionless PDE is solved using extended separation of variables (ESOV) and the results are compared with finite difference method. A dataset has been generated using the ESOV for parameters of batteries. Furthermore, time series analysis is conducted to predict the state of charge (SOC) using long short-term memory (LSTM) networks. The predictions are validated against the ESOV, demonstrating the efficacy of LSTM in accurately forecasting SOC.

## References

[1] Hong, S. Y., Kim, Y., Park, Y., Choi, A., Choi, N. S., & Lee, K. T. (2013). Charge carriers in rechargeable batteries: Na ions vs. Li ions. *Energy & Environmental Science*, *6*(7), 2067-2081.

[2] Chayambuka, K., Mulder, G., Danilov, D. L., & Notten, P. H. (2020). From li-ion batteries toward Na-ion chemistries: challenges and opportunities. *Advanced energy materials*, *10*(38), 2001310.

[3] Chayambuka, K., Jiang, M., Mulder, G., Danilov, D. L., & Notten, P. H. (2022). Physics-based modeling of sodium-ion batteries part I: Experimental parameter determination. *Electrochimica Acta*, *404*, 139726.

[4] Chayambuka, K., Mulder, G., Danilov, D. L., & Notten, P. H. (2022). Physics-based modeling of sodium-ion batteries part II. Model and validation. *Electrochimica Acta*, *404*, 139764.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Impact of Injector Nozzle Variation on HCCI Engine Performance with Juliflora Biodiesel and Hydrogen Using Response Surface Methodology

**S. VENKATESAN**[1*,] **P. RAGHU**[2*]

[1]*Research Scholar, Department of Mechanical Engineering, Sri Venkateswara College of Engineering, Pennalur, Sriperumbudur –602 117, Tamilnadu, India*
[2]*Associate Professor, Department of Mechanical Engineering, Sri Venkateswara College of Engineering, Pennalur, Sriperumbudur –602 117, Tamilnadu, India*
[*1]venkyy1992@gmail.com,[2]praghu@svce.ac.in,

**Keywords**: Hydrogen, Injector nozzle, Response Surface Methodology (RSM), Engine efficiency, Emission control.

Hydrogen, a promising renewable energy carrier, can efficiently complement existing compression ignition diesel engines in dual-fuel configurations with minimal modifications. This study explores the performance and emissions characteristics of Homogeneous Charge Compression Ignition (HCCI) engines fueled by diesel, biodiesel, and a blend of Juliflora Biodiesel (B20) with hydrogen. The research investigates varying injector nozzle configurations (3-hole, 4-hole, and 5-hole) to enhance engine efficiency and reduce emissions. Prosopis Juliflora Biodiesel (B20, 20% biodiesel and 80% diesel) serves as the primary fuel, supplemented with hydrogen at 6 liters per minute through the inlet manifold. Experimental findings show that a 4-hole nozzle at 50% load (B20 + H2 6 LPM) achieves superior atomization, increased brake thermal efficiency, and reduced CO, HC, and smoke emissions compared to other configurations. Response Surface Methodology (RSM) validates these results, confirming optimized parameters for improved performance. The study recommends implementing the 4-hole nozzle for the B20 + H2 blend to optimize fuel-air mixture distribution and combustion efficiency. This research contributes insights into leveraging dual-fuel capabilities and injector nozzle design to advance the efficiency and sustainability of HCCI engines with alternative fuels like Juliflora biodiesel and hydrogen.

References

1. Cai, Y., Zhang, Z., Liu, H., & Lu, X. (2020). Effects of nozzle number on performance and combustion characteristics of a hydrogen direct-injection homogeneous charge compression ignition engine. *International Journal of Hydrogen Energy, 45*(5), 3447-3459. doi:10.1016/j.ijhydene.2019.11.133
2. Lapuerta, M., Armas, O., & Rodríguez-Fernández, J. (2019). Influence of nozzle geometry on the injection of biodiesel fuel in diesel engines. *Renewable Energy, 143,* 380-390. doi:10.1016/j.renene.2019.05.093
3. Agarwal, A. K., & Das, L. M. (2019). Biodiesel development and characterization for use as a fuel in compression ignition engines. *Renewable and Sustainable Energy Reviews, 23,* 383-399. doi:10.1016/j.rser.2013.03.013.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Kinetics and Mechanism for Catalyzed Oxidation of Oxacillin

**YUV RAJ SAHU[1], NARENDRA KUMAR CHAUDHARY[1], AJAYA BHATTARAI[1]**

[1]Department of Chemistry, Mahendra Morang Adarsh Multiple Campus, Tribhuvan University,
Biratnagar, 56613, Nepal

**Keywords**: Oxacillin, Kinetics, Monoperiodatocuprate (III), Equilibrium Constant, Oxidation, Mechanism.

Oxidation of oxacillin has been predicted by monoperiodatocuprate [MPC (III)] at 25°C with 0.10 mol dm$^{-3}$ ionic strength, in an alkaline medium, by Cobalt (III) catalyst and UV/Visible spectrophotometric analysis, for which 1:4 stoichiometry is visible. The reaction products have been recognized using spectral reports from the FT-IR, LC-MS, and spot tests. A pseudo-first order reaction has been confirmed for the oxidant, fractional order for the substrate and alkali, even though Periodate claimed a delaying effect. The primary active species in the alkaline medium, $[Cu(H_2IO_6)(H_2O)_2]$ was discovered to be monoperiodatocuprate [MPC (III)]. The evaluation of activation and thermodynamic parameters is aided by the identification of the catalyzed rate constants, catalytic constant, slow step rate constant, and equilibrium constants. A potential rate constant derivation along with a plausible mechanism that would explain the experimental findings has been put forth and thoroughly examined.

The present research work holds significant importance due to degradation technique by the utilization of diperiodatocupratic (III) oxidation method. Hence the proposed study aims to disclose a novel application in the context of catalysed degradation of non-biodegradable PADs or antibiotics in the aqueous alkaline medium which may be fruitful in the direction of selecting the best and most rapid ways to reduce pollution and in de-activating their uncontrolled growing potentiality in future for the coming generation.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermal Decomposition and Kinetic Study of Chemically Treated Glass Fiber Reinforced Polymer Composites

**ELEDATHU KURIACHAN SACHIN[1], NELSON MUTHU[2], PANKAJ TIWARI[1]***

[1]Department of Chemical Engineering, Indian Institute of Technology Guwahati, Assam, India.
[2]Department of Mechanical Engineering, Indian Institute of Technology Palakkad, Kerala, India.
*Corresponding author: email: pankaj.tiwari@iitg.ac.in

**Keywords**: Glass fibrous composites, TGA, kinetics, catalysis, pyrolysis

Glass fiber-reinforced polymer (GFRP) composites are used extensively in a wide range of industries due to their outstanding mechanical characteristics [1]. However, the resulting waste creates a significant disposal challenge, emphasizing the importance of efficient recycling. Among the different recycling processes, pyrolysis is the most promising thermal treatment method [1]. Catalytic pyrolysis has distinct advantages over conventional pyrolysis while delivering high-quality recovered fibers [1]. This study focuses on the influence of the catalyst on the kinetic and decomposition of the GFRP composites. The catalyst system consists of 20% $ZnCl_2$-Ethanol in which the GFRP specimens are pre-treated at 75˚C for 2 hrs. The TGA analysis of the raw and pre-treated samples was performed at different heating rates from room temperature to 600˚C. The decomposition profile of both samples was plotted in Figure 1(a) and found that there is a reduction of 89.9˚C in the decomposition profile of the pre-treated GFRP. The $Zn^{2+}$ ions link with the C-N bond in epoxy and promote the decomposition of epoxy at lower temperatures [2].

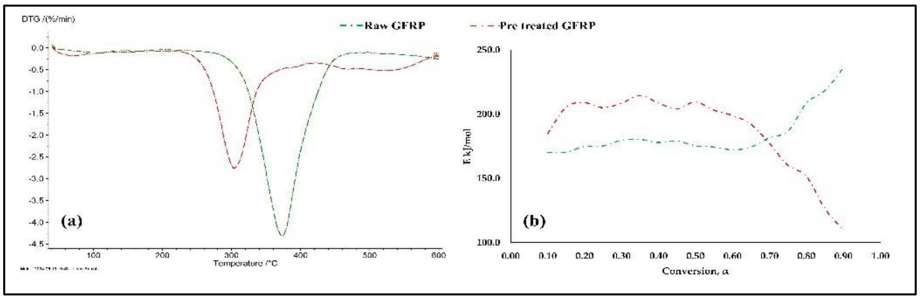


**Figure 1(a)**. DSC and **(b)** E vs. conversion graphs of raw and pre-treated samples

The kinetics of the process were modelled using Friedman's equation to evaluate the kinetic triplets. The calculated activation energy (E) values are plotted in Figure 1(b) for the raw and pre-treated GFRP samples. From the figure, it is clear that the 'E' of the pre-treated sample is higher until the conversion reaches 0.7. It can be attributed to the fact that at lower temperatures $Zn^{2+}$ ions promote higher 'E' reaction pathways. Further product analysis is required to evaluate the mechanisms occurring at lower conversion/temperature levels, aiming to better understand this phenomenon. More results will be presented in the full paper.

**Acknowledgment**
The financial assistance provided by Tata Steel Limited is gratefully acknowledged.

### References

[1] EK Sachin et al., *Journal of Reinforced Plastics and Composites*, **2024**
[2] EK Sachin et al., *Sustainable Environment*. **2023**. Singapore: Springer Nature Singapore.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# From Viscosity to Crystal Growth and Diffusion: A Comprehensive Study of $Ge_{25}Se_{75}$ Amorphous Material Prepared in Different Forms

**JAROSLAV BARTÁK**[1*], **DAVID VACULÍK**[1], **MICHAELA VCELÁKOVÁ**[2], **PETR KOŠTÁL**[2], **JIRI JANCALEK**[3], **MICHAL KURKA**[3], **SIMONA MARTINKVÁ**[1], **JIRÍ MÁLEK**[1]

[1] Department of Physical Chemistry, University of Pardubice, Studentska 573, 53210 Pardubice, Czech Republic
[2] Department of Inorganic Technology, University of Pardubice, Doubravice 41, 53210 Pardubice, Czech Republic
[3] Department of General and Inorganic Chemistry, Faculty of Chemical Technology, University of Pardubice, Studentska 573, 532 10 Pardubice, Czech Republic
*Corresponding author: e-mail: jaroslav.bartak@upce.cz

**Keywords**: viscosity, crystal growth, diffusion, chalcogenide glass, thin films

Chalcogenide materials are widely used in practical applications. These materials, in the form of bulk glasses and thin films, exhibit high transparency and nonlinearities in a broad infrared (IR) region, making them promising materials for IR optics. They show pronounced optical and electronic transport properties changes during switching between amorphous and crystalline states. Therefore, they find the utilization in data storage devices, optical switches, tunable emitters, absorbers, nonvolatile photonics, etc.

It is evident that the chalcogenide amorphous materials need to be prepared in different forms (bulks, fibers, thin films) for various types of practical applications. Therefore, studies of physical properties (such as viscosity, diffusion, thermal properties, etc.) and kinetic phenomena (structural relaxation, crystallization) taking place in amorphous materials must be studied and compared in these sample types to predict their behavior under certain conditions.

The contribution is focused on investigating crystal growth and viscosity in $Ge_{25}Se_{75}$ chalcogenide glass-forming material. Samples were prepared in bulk glass using the classical melt-quench process, and thin films were made using thermal evaporation and solution processing. The study interconnects the information about the structure (found from XRD analysis), crystal growth (followed by infrared microscopy), and viscous flow (measured in the whole range from glass, through undercooled melt, up to melt) to provide detailed knowledge about the crystal growth phenomenon and diffusion in the $Ge_{25}Se_{75}$ amorphous material prepared in different forms.

**Acknowledgments**

This work has been supported by the Czech Science Foundation under grant no. 24-10480S; the Ministry of Education, Youth and Sports of the Czech Republic under grant no. LM2023037; by the Internal Grant Agency of the University of Pardubice under Selected Research Teams program of the University of Pardubice and under SGS grant no. SGS_2024_007.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Exploring dielectric and AC conduction characteristics in elemental selenium glass modified with silver halides

A. KUMAR[1], V. SARASWAT[1], N. MEHTA*[1]

[1]Department of Physics, Banaras Hindu University, Varanasi 221005, India
*Corresponding author: e-mail: dr_neeraj_mehta@yahoo.co.in

**Keywords**: Glass-ceramic, Dielectric constant, Dielectric loss, AC conductivity, Density of states

In this research work, we have examined the influence of silver halide doping on the dielectric dispersion and AC conduction of elemental selenium. The in-depth investigation shows that when the dopant silver halides are incorporated, there are noticeable changes in the parent selenium's dielectric constant ($\varepsilon'$), dielectric loss ($\varepsilon''$), and AC conductivity ($\sigma_{ac}$). When we frame the discussion of the obtained results with the relevant transport models, we found that in pure selenium and $Se_{95}(AgI)_5$, conduction is primarily due to polaron hopping and follows the correlated barrier hopping (CBH) model. In contrast, $Se_{95}(AgBr)_5$ predominantly exhibits non-overlapping small polaron tunnelling (NSPT). Interestingly, $Se_{95}(AgCl)_5$ demonstrates both NSPT and CBH conduction mechanisms, depending on the temperature range: NSPT is dominant between 303 K and 313 K, while CBH prevails from 318 K to 338 K. Additionally, our findings revealed the presence of both the Meyer–Neldel rule (MNR) and its reverse in the prepared silver halide chalcogenide alloys. The best optimization of dielectric constant and loss is observed for silver iodide as compared to silver chloride and silver bromide. Comparison with other silver-containing chalcogenide glasses indicates the better dielectric performance of the present silver halides containing selenium.

**References**

[1] V. Saraswat, S. K. Pal, A. Dahshan and N. Mehta. *J. Non-Cryst. Solids*, 617 (**2023**) 122487.
[2] S. R. Elliott. *Philos. Mag. B*, 37 (**1978**) 553–560.
[3] N. Goyal, A. Zolanvari and S. K. Tripathi. *J. Mater. Sci.: Mater. Electron.*, 12 (**2001**) 523–526

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Experimental investigation of hybrid nanoparticles based eutectic phase change materials for efficient thermal energy storage.

**ANKUR ARUN BHANSALI[1]*, DEBABRATA PANDA[2], KRUNAL MADHUKAR GANGAWANE[1]**

[1]Department of Chemical Engineering, Indian Institute of Technology Jodhpur, Rajasthan, India
[2] Department of Chemical Engineering, NIT Rourkela
*Corresponding author: e-mail: bhansaliankur@iitj.ac.in

**Keywords**: Thermal Energy Storage, Eutectic Phase change materials, Hybrid Nanoparticles, Heat augmentation

In recent years, energy sustainability is a major concern. To overcome this, the thermal energy system (TES) has become one of the most important components to increase the overall system efficiency of various industrial applications. Thermal energy can be stored mainly by three basic forms: sensible heat, latent heat and chemical heat storage. Out of the three, Latent heat thermal energy storage systems (LHTES) have higher potential due to its high energy storage density where the energy is stored at the phase change transition temperature. Phase change materials (PCMs) have been found suitable for LHTES due to various ranges of latent heat and melting points. The limitations of PCM based LHTES is the lower thermal conductivity of organic and hydrated salts. There is a very limited study on the eutectic phase change materials (EPCM) and their combination with hybrid nanoparticles (NPs) PCM based heat exchangers can be improved using a mixture of various phase change materials and nanoparticle dispersion. An experimental setup of shell and tube heat exchanger was made to study the effect of eutectic mixture of paraffin wax and peg-6000 and then with dispersion of hybrid nanoparticle combination of Graphene Oxide and Multi walled carbon nanotubes. Various characterization techniques were performed of the EPCM+NPs combination to find the structure, composition, morphology, and other relevant properties like latent heat and thermal conductivity. The EPCM+NPs melting behavior is studied by varying different parameters.

**References**

[1] Maher H, Rocky KA, Bassiouny R, Saha BB. Synthesis and thermal characterization of paraffin-based nanocomposites for thermal energy storage applications. Thermal Science and Engineering Progress. 2021 May 1;22.
[2] Lu Z, Wang S, Ying H, Liu B, Jia W, Xie J, et al. Preparation and thermal properties of eutectic phase change materials (EPCMs) with nano graphite addition for cold thermal energy storage. Energy. 2024 Mar 1;290.
[3] Sharma A, Tyagi V V., Chen CR, Buddhi D. Review on thermal energy storage with phase change materials and applications. Vol. 13, Renewable and Sustainable Energy Reviews. 2009. p. 318–45.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Graphene Quantum Dots as Ratiometric Fluorescent Sensor for Lactic Acid

**Seikh Asif[1], Kamalika Sen[1]***

[1]Department of Chemistry, University of Calcutta, 92, APC Road, Kolkata 700009, India

*email: kamalchem.roy@gmail.com

**Keywords**: Ratiometric fluorescence, Graphene Quantum Dots, Lactic acid

Research and clinical diagnosis stand to gain significantly from the development of a very sensitive fluorescence probe for biomolecule detection. With regard to their low toxicity, excellent water dispersibility, biocompatibility, chemical inertness, photostability, ease of synthesis, and exceptional photoluminescence properties, Graphene Quantum Dots (GQDs) are novel zero-dimensional graphitic nanomaterials that hold great promise for use in biological sensing [1]. In this work, GQDs were synthesized, characterized, and explored as a fluorophore in sensitive determination of lactic acid. In the present study, GQDs were prepared by pyrolysis of aspartic acid in glycerol medium. The characterization of the prepared GQDs was investigated using Fourier-transformed infrared (FT-IR) spectroscopy, Transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), Dynamic light scattering (DLS) and Zeta potential measurements. A ratiometric fluorescence probe towards lactic acid with a good linear range of 7.389-65.217 μM and limit of detection (LOD) of 5.846 μM is developed. The development of ratiometric fluorescence instead of monochromatic fluorescence improves the stability and accuracy of the detection method. The developed probe was applied to lactic acid detection in human serum with satisfactory results, indicating that the probe has enormous potential in clinical practice. Moreover, the sensing capacity of the GQDs was further validated in presence of various interfering agents such as ascorbic acid, citric acid, nitrate, glucose, cholesterol and uric acid in serum medium.

### Reference

[1] Y. Dong, J. Shao, C. Chen, H. Li, R. Wang, Y. Chi, X. Lin, G. Chen, *Carbon* 50 (**2012**) 4738−4743.

# Deep-Ultraviolet (DUV) nonlinear optical (NLO) crystals: An application in Photonic Technologies

**BISWAJIT DALAI[1*], SARAT KUMAR DASH[2*]**

1Department of Physics, School of Sciences, Gandhi Institute of Engineering and Technology University, Gunupur-765022, Odisha, India
2Department of Physics, Regional Institute of Education (NCERT), Bhubaneswar, Odisha– 751022, India
*Corresponding author: e-mail: biswajit@giet.edu (BD), skdash59@yahoo.com (SKD)

**Keywords**: NLO, SHG, band gap, LIDT, birefringes

In the past decades, great efforts have been focused on the search for new nonlinear optical (NLO) materials that can work from deep-UV (wavelengths below 200 nm) spectral regions to even far-infrared regions. An overview on deep-ultraviolet nonlinear optical (DUV NLO) materials was summarized from an extensive literature survey and analyzed the results. Deep-UV NLO crystals are of worldwide interest for the generation of coherent light with wavelength below 200 nm by the direct second-harmonic generation (SHG) output from solid-state lasers. Alkali-/alkaline elements were basically used for NLO Crystals. Different charges/size combinations in the mixed cation compounds have different influences on the packing of anions and hence on their structures and properties. The crystals with units of phosphate (-$PO_4$) and sulphate (-$SO_4$) generally exhibit poor polarizability and optical anisotropy, which results in weak NLO effect and birefringence. The nonlinear optics has been utilized for frequency conversion phenomena in various fields of modern optics and laser technology, like all solid-state lasers, ultrafast lasers, spectrometers, optical storage, electro-optic modulation, photorefractive effect and computing. NLO technology is the most mature method to extend wavelength limits of practical laser sources. Practical NLO technologies depend heavily on the availability of NLO crystals. These DUV lasers have importance in cutting-edge technologies such as medical, micromachining, lithography, photochemistry, spectroscopy, and microscopy. Beryllium-based borate structures are still ideal candidate materials system for DUV NLO crystals. An ideal DUV / UV NLO Crystal with superior comprehensive performance is very challenging.

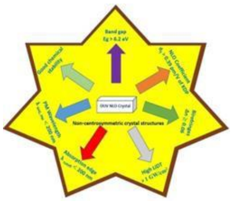


Fig. 1: Various parameters used for the characteristics of DUV NLO Crystals

**References**

[1] [Y.G. Chen, X. Yu, Y. Guo, Y. Xue, X. Hao, X. Yao and X.M. Zhang, *J. Alloys Compd.*, 896 (**2022**) 162975.
[2] F. Wang, X.N. Yao, Y. Guo, L.G. Yang, Y.G. Chen and X.M. Zhang, *J. Solid State Chem.*, 301 (**2021**) 122333.
[3] Z. Dai, Y.G. Chen, Y. Guo, F. Wang, Y. Y. Yang and X. M. Zhang, *Inorg. Chem.*, 60 (**2021**) 11214.
[4] M. Mutailipu, K.R. Poeppelmeier and S.L. Pan, *Chem. Rev.* 121 (**2021**) 1130.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Generalized interface reaction kinetic models for heterogeneous contracting processes

**LUIS A. PÉREZ-MAQUEDA[1*], JUAN ARCENEGUI-TROYA[2], PEDRO E. SÁNCHEZJIMÉNEZ[1], ANTONIO PEREJÓN[1,3]**

[1]Instituto de Ciencia de Materiales de Sevilla (CSIC-USE) Sevilla 41092, Spain
[2] Departamento de Electricidad y Electromagnetismo, Universidad de Sevilla, Sevilla 41012, Spain
[3]Departmento de Química Inorgánica, Universidad de Sevilla, Sevilla 41012, Spain *Corresponding author: e-mail: maqueda@icmse.csic.es

**Keywords**: Heterogenous process; Interface kinetic model; Kinetics; Non-ideal kinetic model; Solid-state processes

Kinetic analysis of heterogeneous processes implies getting reliable kinetic parameters that properly describe the process. Ideal kinetic models are used to gain insight about the process mechanism. These models are constrained by a number of assumptions rarely met in real systems. Thus, in the case of the commonly used contracting (or interface) kinetic models, For example, for the R2 ideal kinetic model, it is assumed a perfect cylindrical contraction in the radial direction, while contraction in the direction of the axis of the cylinder is not taken into consideration. Besides, for the R3 model, it is supposed contraction in all three directions of space for perfect spheres or cubes of identical dimensions. We have reanalysed contraction models considering different geometries, such as cylinders with different aspect ratios or rectangular cuboids and find mathematical equations for such processes. A new generalized interface reaction equation that cover all studied cases is presented. This new equation fits all studied cases including different geometries and particle size distributions. Presented equations are applied to real experimental data, providing a very accurate description of the studied processes.

# Exploring Compensation Effect and Conduction Mechanism in Current-Voltage Characteristics for Binary ST system and Ternary STTM (i.e., doped transition metals Fe, Co, Ni, Cu) system

**NISHA KUMARI[1], VISHNU SARASWAT[2], NEERAJ MEHTA[1]***

[1,2]Department of Physics, Banaras Hindu University, Varanasi-221005, India
*Corresponding author: e-mail: dr_neeraj_mehta@yahoo.co.in

**Keywords**: Transition metal chalcogenides, Electrical properties, Resistive Switching, Threshold Voltage, Poole-Frenkel effect

## Abstract

The investigation analyzed the current-voltage characteristics and d.c. electrical conductivity of $Se_{80}Te_{20}$ (ST) and $Se_{78}Te_{20}TM_2$ (STTM, where TM = Fe, Co, Ni, Cu) glassy thin pellets. All samples with nearly identical disc-shaped specimens were employed to investigate the current-voltage (I - V) characteristics at various temperatures below the glass transition temperature within these pellets, focusing on understanding their behavior relative to multicomponent system. Upon analyzing the experimental data, our investigation reveals the occurrence of resistive switching in both the parent and doped transition metal chalcogenides system. A compensatory effect was observed in the thermal activation involved in the resistive switching of these samples. Analysis of the experimental data indicates the presence of space charge-limited conduction in both binary and ternary alloys. This is evident from the ln ($I/V$) versus $V$ curves, which exhibit nearly straight-line with decreasing slopes at high temperature range with a high correlation coefficient. Linear relationships between $lnI$ and $V^{1/2}$ were observed across both low and high-voltage ranges. These findings were elucidated using the Pool-Frenkel mechanism. While the I - V characteristics display ohmic behavior at lower voltages, transitioning to non-ohmic behavior at higher voltages is attributed to voltage-induced temperature effects.

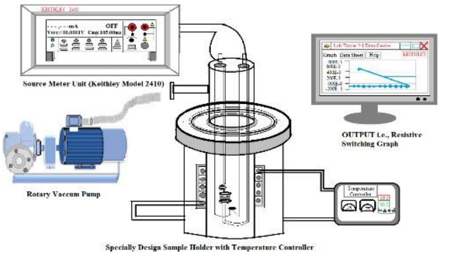


Fig.1: Setup for I-V characteristics

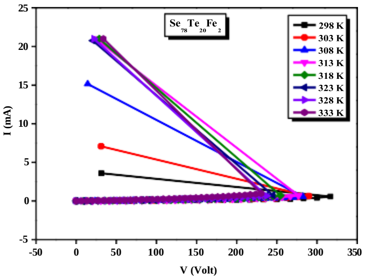


Fig. 2 Resistive switching for $Se_{78}Te_{20}Fe_2$

### References

[1] N. Mehta, *Journal of Scientific and Industrial Research*, 65 (2006) 777–786.
[2] S. Agarwal, D. K. Dwivedi, P. Lohia, *Journal of alloys and Compounds* 983 (2024) 173773.

**T3- OP 08**

# Tailoring of Selenium Nanocomposite Properties: Unveiling the Role of rGO/Graphite in Dielectric, Mechanical, and I-V Characteristics

**SACHIN KUMAR YADAV [1], , NEERAJ MEHTA[1]***

[1]Department of Physics, Banaras Hindu University, Varanasi-221005, India
*Corresponding author: e-mail: dr_neeraj_mehta@yahoo.co.in

**Keywords**: Reduced graphene oxide (rGO), Dielectric properties, Hopping Mechanism, Electrical transport, Mechanical properties

## Abstract

This work examines the dielectric, electrical, and microhardness properties of melt-quench prepared graphite@rGO#Selenium nanocomposites. Dielectric properties of the NCs have been investigated in the frequency range from 100 Hz to 500 kHz and in the temperature range from 303 K to 333 K. According to frequency-dependent AC conductivity studies, the prepared NCs follow the correlated barrier hopping (CBH) model. The permittivity increases due to interfacial polarization and the expansion of the microcapacitor network. The frequency-dependent conductivity spectra follow Jonscher's universal power law. The electrical conductivity of NCs is found to be thermally activated and also we have elucidated the activation energy, the hopping distance, and the maximum barrier height of the NCs. The dielectric constant and loss of Se:rGO NCs are 29.54 and 0.14 compared to bare selenium (21.72, 5.14), at 1 kHz, respectively. This suggests that the Se:rGO NC is a promising dielectric with a high dielectric constant and low dielectric loss. The enhanced mechanical properties could be attributed to the increased crystallinity of the pure selenium matrix and rGO-reinforced NC. This study has tried to enlighten the behavior of relaxation and conduction mechanism of graphite/rGO reinforced selenium NCs at different temperatures.

**References**

[1] A.J. Marsden, D.G. Papageorgiou, C. Vall´es, A. Liscio, V. Palermo, M.A. Bissett, R.J. Young, I. A. Kinloch (2018). *2D Materials*, 5(3), 032003.
[2] P. Kumar, S. Penta, S.P. Mahapatra (2019). *Integrated Ferroelectrics*, 202(1), 41-51.

T3- OP 09

# A 2D Supramolecular Cu (II) complex with 4,4$^{/}$diaminodiphenylsulphone: Synthesis, spectroscopic characterizations, crystal structure and its biological activities

**Shamjetshabam Sumitkumari Devi**[1], **R.K. Hemakumar Singh**[2 *]

[1,2] Department of Chemistry, Manipur University, Canchipur-795003, Manipur, India
[*] Corresponding author: e mail: rkhemakumar@manipuruniv.com

**Keywords**: copper (II) complex, 4,4$^{/}$-diaminodiphenylsulphone, monoclinic,2D supramolecular, biological activities

A Cu (II) complex [Cu (DDS)$_2$ (H$_2$O)$_2$Cl$_2$] (DDS= 4,4$^{/}$ -Diaminodiphenyl sulphone) was successfully synthesized using methanol by stirring at room temperature. The complex is characterized using SC-XRD, IR, UV and thermogravimetric analysis. Single crystal X-ray analysis of 1 indicates a distorted octahedral coordinated Cu$^{2+}$ centre with two molecules of DDS, two chlorine ions and two water molecules in the complex. The two chlorine atoms (Cl1 and Cl2) form intermolecular hydrogen bonding. The complex crystallizes in monoclinic space group P2$_1$/n forming a 2D polymeric supramolecular architech through H- bonding. The presence of π…π intermolecular stacking between the aromatic rings was confirmed by SC-XRD. Complex 1 shows appreciable biological activities.

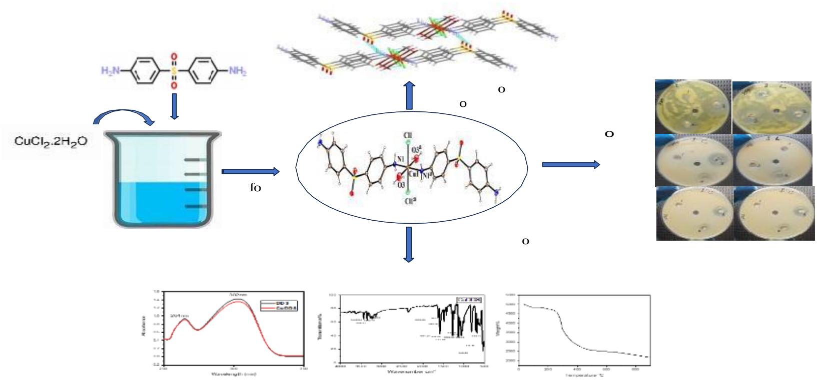


Fig 1: Scheme for synthesis, characterizations and biological study

**References**

[1]. S. Mendiratta, C. Hua Lee, S. Ying Lee, et al. *Molecules*.20 (**2015**) 8941.
[2]. G.M. Sheldrick, *Acta Crystallographe.A*.64 (**2008**) 112- 116.
[3]. J. Mastern, N. Baumer, G.Farnandez.*J.Am.Chem.Soc*.143(**2021**) 7164-7175

**T3- OP 10**

# Fabrication and analysis of Aluminium based Metal Matrix Composite with Carbon Nano Tube (CNT) as reinforcement

**SREEKUMAR E.N.**[1, 2*], **M.S SENTHIL SARAVANAN**[2]

1 Research Scholar, APJ Abdul Kalam Technological University, Thiruvananthapuram,
2 Department of Mechanical Engineering, Sree Buddha College of Engineering, Kerala
* Corresponding author: e-mail: sreekumar.rit@gmail.com

**Keywords**: Thermo Gravimetric Analysis (TGA), Differential Thermal Analysis (DTA), Microhardness, Microstructure

Metal matrix composites have gained significant attention in recent years due to their enhanced thermal and mechanical properties compared to conventional materials. Aluminium is one of the lightest and mostly used structural material due to their favourable properties. The incorporation of Carbon Nanotubes (CNT) enhances the thermal as well as mechanical properties, hence the performance of metal matrix composites. The thermal and mechanical behavior of CNT reinforced Al-Cu composite fabricated through powder metallurgy processing is discussed in the proposed work. The processing involves the preparation of the composite powder, with careful dispersion of CNTs within the aluminium matrix. The microstructure of the composite was also analysed.

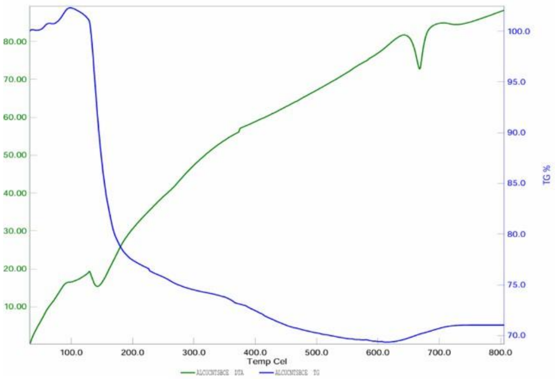


Fig. 1: TG/DTA curve of composite sample 1

**References**

[1] L Sridhar Karthic R. Narayanan, "Processing and characterization of MWCNT reinforced aluminum matrix composites", J Material Science ,2019.

[2] M.S. Senthil Saravanan, S.P. Kumaresh Babu, K. Sivaprasad, M. Jagannatham; Technoeconomics of carbon nanotubes produced by open air arc discharge method; International Journal of Engineering, Science and Technology Vol. 2, No. 5, 2010, pp. 100-108

# Specific heat measurement of refractory metals and their binary alloys at temperatures above 1500°C

**VEERARAAHAVAN R S[1]*, MONDAL TK[1]**

[1]Indian Institute of Science, Bangalore 560012, India
*Corresponding author: e-mail: veeraraahava@iisc.ac.in

**Keywords**: thermal analysis, sub second calorimetry, specific heat capacity, thermophysical properties

The experimental data on specific heat capacity of pure substances and alloys at temperatures above 1500°C are important for industrial applications. This work aims to develop an empirical correlation of specific heat as a function of temperature for novel alloys between 1500°C and 1800°C using experimental results. The pulse heating method[1], one of the specific heat measurement techniques advantageous at high temperatures, will be adopted to develop the specific heat measurement setup with in-situ alloy formation. The setup will be validated by measuring standard reference materials and comparing the results with literature. Subsequently, experimental data of new alloys will be measured. The specific heat data of molybdenum is shown in Figure 1 and compared with the literature[2].

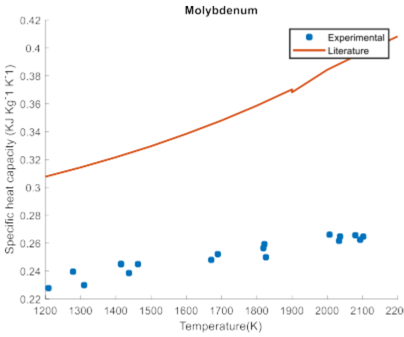


Fig. 1: The specific heat capacity of molybdenum vs temperature

The experimental setup involves the sample holder, made of molybdenum metal with an optimized thickness of 0.3mm. It is placed inside a vacuum chamber to minimize convection loss and oxidation. A lead acid battery bank with a charging and discharging unit supplies a current of 500A to 800A, ensuring rapid joule heating of the sample holder. The temperature of the sample is measured using a Fluke infrared pyrometer. Voltage across the sample is measured using knife edge probes, while current is measured with a 0.15mOhm shunt resistor. Sensor outputs are connected to an NI-DAQ 6215 for data acquisition and control using LabVIEW, and post-processed in MATLAB to calculate the specific heat.

## References

[1] A. Cezairliyan, J. Res. Natl. Bur. Stand., Sect. C 75C, 7 (1971).
[2] Chase, M.W., Jr. J. Phys. Chem. Ref. Data, Monograph 9, 1998, 1-1951.

**T3- OP 12**

# Optimizing Phosphonium-Based Ionic Liquid Electrolytes for Enhanced Supercapacitor Performance

**P. Ghorpade[1]*, G. K. Sharma[1], S. S. Terdale[1*]**

[1]Department of Chemistry, Savitribai Phule Pune University, Pune 411007, India
e-mail: santosh.terdale@unipune.ac.in

**Keywords**: Ionic liquid, graphene oxide, electrolyte, supercapacitor

To increase energy efficiency and satisfy the global demand for sustainable energy, rapid developments in long-lasting, highly efficient, and effective energy resources are required. Although a great deal of research is focused on improving electrode materials for Electric Double-Layer Capacitors (EDLCs), electrolytes play a crucial role in determining specific capacitance and the operational range of energy storage devices. In response to this urgent need, research on electrolytes is becoming increasingly focused. This study focuses on the synthesis and characterization of two phosphonium-based ionic liquids, Tributyltetradecylphosphonium bis(trifluoromethylsulfonyl)imide $[P_{14,4,4,4}][NTF_2]$ and Tetrabutylphosphonium bis(trifluoromethylsulfonyl)imide $[P_{4,4,4,4,}][NTF_2]$, and their application as electrolytes in supercapacitors. The electrolytes were evaluated for their electrochemical performance in combination with graphene oxide (GO) and reduced graphene oxide-nickel oxide (RGO-NiO) composite materials serving as working electrodes.

The synthesis of $[P_{14,4,4,4}][NTF_2]$ and $[P_{4,4,4,4,}][NTF_2]$ involved a systematic approach, including the selection of precursors, reaction conditions, and purification methods, resulting in high purity and yield. Characterization techniques such as nuclear magnetic resonance (NMR) spectroscopy, Fourier-transform infrared (FTIR) spectroscopy, and thermal analysis were employed to explain the chemical structure, purity, and thermal stability of the synthesized ionic liquids.

The electrochemical performance of the supercapacitors was investigated using cyclic voltammetry (CV), galvanostatic charge-discharge (GCD) measurements, and electrochemical impedance spectroscopy (EIS) and will be presented in detail.

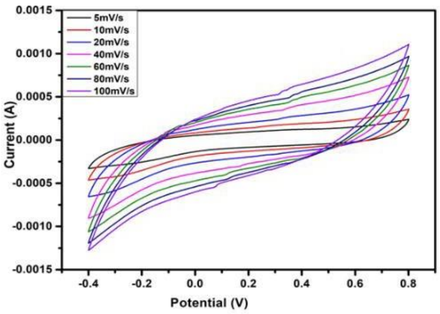


**Fig. 1**: CV analysis of rGO-NiO in 0.2 M $[P_{4,4,4,4,}][NTF_2]$

**References**

[1] Ray A, Saruhan B. *Materials*, 14 (11) (**2021**) 2942.
[2] Guo B, Niu M, Lai X, Chen L. *Glob Energy Interconnect*, 1(1) (**2018**) 79–86.

# Investigation of plasma pyrolysis system for different biomass: An experimental and thermodynamic study

**SIDHARTHA SONDH[1], KANGANA P. BHATT[1], DARSHIT S. UPADHYAY[1]*, SANJAY PATEL[1], RAJESH N. PATEL[1]**

[1]Mechanical Engineering Department, Institute of Technology, Nirma University, Ahmedabad – 382481, Gujarat India
[2]Chemical Engineering Department, Institute of Technology, Nirma University, Ahmedabad – 382481, Gujarat India
*Corresponding author: e-mail: darshit.upadhyay@yahoo.com, darshit.upadhyay@nirmauni.ac.in

**Keywords**: Biomass; Plasma pyrolysis; Thermochemical conversion; Experimental; Thermodynamic analysis

The present study critically offers the biomass/solid waste conversion pathway using plasma pyrolysis technology. Plasma pyrolysis is a thermo-chemical conversion process where carbonaceous feedstock is heated at a very high temperature in an oxygen deficit atmosphere to generate good-quality syngas. In this work, experiments were carried out in 0.5 TPD continuous (thermal) plasma arc pyrolysis with three different biomass: Sawdust (SD), Wood chips (WC), and Rice husk (RH). To compare the data, the electrical power input (12kW), reaction temperature (800℃), and feed rate (20kg h-1) were maintained throughout the experiments. The combustible content (H2, CO, $CH_4$) in the SD, WC, and RH syngas was observed to be 94.5, 94.1, and 88.50%. The cold gas efficiency was found to be at a maximum RH of around 65%. It was observed to be 23% and 37% more than SD and WC, respectively. The Specific Fuel Consumption (SFC) for SD was obtained to be 2 kg kWh-1, which is comparatively better than the other feedstocks. The H2/CO ratio for both the SD and WC was found to be around 1.85, and that of RH was 1.52. Thermodynamic analyses such as mass, energy, and exergy analyses were also carried out, and good agreement was found between input and output groups. Overall, SD is preferred over other selected feedstock in an existing plasma pyrolysis system due to its appreciable cold gas efficiency and lower SFC is the major conclusion of the present study.

**References**

[1] Silpa Kaza, Lisa Yao, Perinaz Bhada-Tata, F.V.W. (2018). What a Waste 2.0: A Global Snapshot of Solid Waste Management to 2050 (World Bank Publications).

[2] Wang, X., Lv, W., Guo, L., Zhai, M., Dong, P., and Qi, G. (2016). Energy and exergy analysis of rice husk high-temperature pyrolysis. Int. J. Hydrogen Energy 41, 21121–21130. 10.1016/j.ijhydene.2016.09.155.

[3] Lu, J.S., Chang, Y., Poon, C.S., and Lee, D.J. (2020). Slow pyrolysis of municipal solid waste (MSW): A review. Bioresour. Technol. 312, 123615. 10.1016/j.biortech.2020.123615.

[4] Dincer, I. (2002). Technical, environmental and exergetic aspects of hydrogen energy systems. Int. J. Hydrogen Energy 27, 265–285. 10.1016/S0360-3199(01)00119-7.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Experimental Investigation of Polycyclic aromatic hydrocarbons (PAHs) Emissions from Gasoline Direct Injection Engines Using Biofuels

**ASHI DUTTA*, PRAVESH CHANDRA SHUKLA**

Indian Institute of Technology Bhilai, Durg 491002, India
*Corresponding author: e-mail: ashidutta@iitbhilai.ac.in

**Keywords** GDI (Gasoline Direct Injection) Engine, Biofuels, PAH (Polycyclic Aromatic Hydrocarbon)

Polycyclic aromatic hydrocarbons (PAHs) are widely recognised for their significant health and environmental risks, primarily due to their carcinogenic and genotoxic properties [1]. This study aims to identify and quantify the levels of polycyclic aromatic hydrocarbons (PAHs) in the particulate matter emitted by gasoline direct injection (GDI) engines when using Biofuels and its blends. The test engine used in this study is a 199.5CC single cylinder GDI engine with a bore of 72mm and a stroke of 49mm. The aim of this study is to investigate the release of polycyclic aromatic hydrocarbons (PAHs) from gasoline direct injection (GDI) engines in different operating conditions, including changing engine loads, speeds, and fuel injection techniques, utilising different types of biofuels and their blends. A previous study indicated that the utilisation of Methanol (a Biofuel) blended gasoline can result in an 80% reduction in PM Emission when utilising M15 (a blend consisting of 15% Methanol) [2]. The present study aims to optimise the GDI Engine in relation to Biofuel and engine parameters. Moreover, this study will offer essential information on the mechanisms behind the formation of polycyclic aromatic hydrocarbons (PAHs) and the impact of engine parameters on emission levels. The analysis technique involves the collection of particle emissions samples, followed by the extraction of polycyclic aromatic hydrocarbons (PAHs) from these samples. The extracted PAHs are then subjected to investigation using high-performance liquid chromatography (HPLC). These findings highlight the significance of strict worldwide emission regulations and enhanced combustion technologies in mitigating the environmental and public health impacts of PAHs.

### References

[1] Kim, Ki-Hyun, Shamin Ara Jahan, Ehsanul Kabir, and Richard JC Brown. "A review of airborne polycyclic aromatic hydrocarbons (PAHs) and their human health effects." *Environment international* 60 (2013): 71-80.

[2] Hong, Wei, Chao Yuan, Fangxi Xie, Yan Su, and Jing Chen. "Particulate matter and particle-bound PAHs emissions from gasoline direct injection (GDI) engine with methanol-gasoline blended fuel during start." International Journal of Automotive Technology 19 (2018): 717-726.

**T4- OP 03**

# Coal bottom ash as an effective catalyst for biomass gasification

**ARJUN C P**[1*], **ARUN P**[1]

[1]Department of Mechanical Engineering, National Institute of Technology, Calicut, Kerala 673601, India
*Corresponding author: e-mail: arjun_p220075me@nitc.ac.in

**Keywords**: coal bottom ash, gasification, energy, biomass, syngas

In gasification, biomass materials are heated to 800 °C to 900 °C to produce a gas mixture rich in hydrogen and carbon monoxide known as synthesis gas or syngas. Catalysts can significantly influence the gasification process, improving the reaction efficiency, gas quality and operational flexibility. This study investigated the use of coal bottom ash sourced from an Indian thermal power plant as a biomass gasification catalyst. Coal bottom ash contains compounds like silicon dioxide, alumina, iron oxides, and calcium oxide and is also not prone to sintering. Silicon dioxide can supplement as a bed material, alumina helps in the cracking of large hydrocarbons like tar, iron oxide enhances syngas production and helps to reduce tar [1, 2]. From the characterization study using EDS, XRF and XRD, it was found that the coal bottom ash had presence of silicon dioxide ($SiO_2$), aluminum oxide ($Al_2O_3$), calcium oxide (CaO), iron oxide ($Fe_2O_3$), magnesium oxide (MgO), potassium oxide ($K_2O$) and titanium oxide ($TiO_2$) in it. From the SEM image obtained, it was found that the surface roughness of the coal bottom ash was reasonably high.

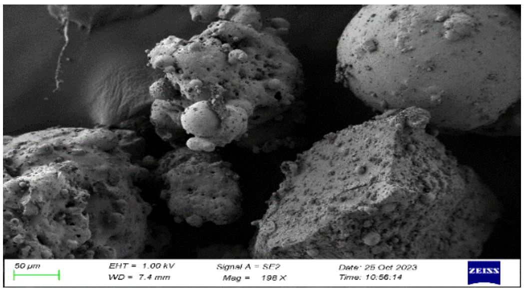


Fig. 1: SEM image of coal bottom ash

The effectiveness of coal bottom ash as a gasification catalyst depends on its specific characteristics and gasification process parameters. Further studies are essential to optimize its use and understand its full potential for enhancing gasification efficiency and product quality, particularly in the Indian context.

## References

[1] M. Hussain, L. Dendena Tufa, S. Yusup, and H. Zabiri, “Characterization of Coal Bottom Ash &its Potential to be used as Catalyst in Biomass Gasification,” Materials Today Proceedings, 16 (2019), pp. 1886-1893.

[2] A C M Loy, S Yusup, M K Lam, B L F Chin, M Shahbaz, A Yamamoto, M N Acda, “The effect of industrial waste coal bottom ash as catalyst in catalytic pyrolysis of rice husk for syngas production,” Energy Conversion and Management, 165 (2018), pp. 541–554.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Impact of Acylthiourea Based Rhodium Complexes on Proteolytic Activity and Conformational Stability of α-chymotripsin

**DEEPAK CHAHAR, PANNURU VENKATESU***

Department of Chemistry, University of Delhi, 110007
*Corresponding author: e-mail: venkatesup@hotmail.com

In this research study, a series of four acylthiourea ligands and their corresponding rhodium (III) pentamethylcyclopentadienyl complexes, designated as Rh1, Rh2, Rh3 and Rh4 were successfully prepared. Through meticulous analysis of the spectroscopic data, it was convincingly established that the acylthiourea ligands served as neutral and monodentate ligands in their interaction with the Rh (III) ions. Specifically, the spectroscopic evidence confirmed that the sulfur (S) atoms within the acylthiourea ligands formed coordinated bonds with the Rh (III) ions. This crucial finding elucidates the specific coordination mode and binding interactions between the ligands and the central Rh (III) metal ion, which has been seldom investigated. The biomolecular interactions of the all the Rh complexes with α-chymotripsin have also been studied in detail using various spectroscopic and microscopic methods, such as UV-Visible spectroscopy, Fluorescence spectroscopy, FTIR spectroscopy, Raman spectroscopy, Dynamic light scattering (DLS). Thermal denaturation study was also performed using Fluorescence spectroscopy. Further, our results deliver that all the Rh complexes are able to interact with αchymotripsin with maintenance of structural stability as well as enzymatic activity of enzyme. Further, the proteolytic activity of α-chymotripsin in presence of all Rh complexes increases to higher extent.

## References

[1] Bisht, M.; Mondal, D.; Pereira, M. M.; Freire, M. G.; Venkatesu, P.; Coutinho, *Green Chem.*, 19 (**2017**) 4900−4911

[2] Kumar, P. K.; Bisht, M.; Venkatesu, P.; Bahadur, I.; Ebenso, *J. Phys. Chem. B,* 122 (**2018**) 10435−10444

T4- OP 05

# Green synthesis of copper oxide nanoparticles using *Hedhycium rubrum*, antimicrobial assay and anticancer assay against A549 and HeLa cell lines

**Ksh Sangeeta Devi**[1*], **N.Rajen Singh**[2]

[1]Department of Biotechnology, Jadonang Memorial College,Noney795159,India
[2]Department of Chemistry, Manipur University,Canchipur795003,India
[*]Corresponding author:e.mail:kshetrimayumsangeeta@gmail.com

**Keywords**: antibacterial, anticancer, green synthesis NPs, ecofriendly

The synthesis of nanoparticles using green synthesis method is budding into an important approach in nanotechnology as an ecofriendly and convenient method [1,2] The green synthesized of CuO NPs using *Hedhycium rubrum* (medicinal plants from Manipur) rhizome aqueous extract as a novel reducing and stabilizing agent. The green synthesized CuO NPs were characterized by XRD, FT-IR, SEM, EDX and UV-Vis Spectrophotometer**.** antimicrobial assay and anticancer assay against A549 and HeLa cell lines. The green synthesized CuO NPs consisted of uniformly distributed spherical-shaped particles in aggregated form and monoclinic crystal structure. The absorption spectra with a distinct peak centered 290 nm indicates the presence of CuO NPs. In this, antibacterial activities of the green synthesized CuO NPs against 5 UTI causing bacteria, *Klebsiella pneumonia* shows the highest zone of inhibition more than that of standard (Gentamicin). In anti-cancer activity assay the IC50 is found to be 60.691ng/µL and 2.476 ng/µL for A549 and HeLa cells respectively, we can see that the IC50 value is lower in HeLa cell line which means that the HeLa cells are more susceptible to the compound then A549 cells.

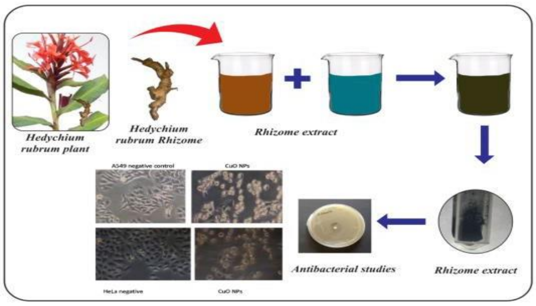


Fig.1: Schematic presentation of the experiment.

**References**

[1] P. Raveendran, J. Fu and S.L. Wallen, *Green Chem*., 8 (**2006**) 34-38.

[2] P. Magudapathy, P. Gangopadhyay, B.K. Panigrahi, K. G. M. Nair and S. Dhara. *Condens, Matter*. 299 (**2001**) 142-146.

[3] Shi, L.-B., Tang, P.-F., Zhang, W., Zhao. *et alTrop. J. Pharm. Res*. 16 (**2017**) 185-192.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Optimization And Comparison of Various Biodiesels Using Response Surface Methodology and Machine Learning Techniques

**E.SOMA SIVA[1],E.GURUNATH RAJ[1],P.RAGHU[2] S.VENKATESAN[3]**

[1*1]*Undergraduate Students,Department of Mechanical Engineering, Sri Venkateswara College of Engineering, Pennalur, Sriperumbudur –602 117, Tamil Nadu, Indi*a
[2] *Associate Professor, Department of Mechanical Engineering, Sri Venkateswara College of Engineering, Pennalur, Sriperumbudur –602 117, Tamil Nadu, India*
[3]*Research Scholar, Department of Mechanical Engineering, Sri Venkateswara College of Engineering, Pennalur, Sriperumbudur –602 117, Tamil Nadu, India*
[1*]2021me0427@svce.ac.in, [1] 2021me0518@svce.ac.in, [2]praghu@svce.ac.in,
[3]venkyy1992@gmail.com,

**Keywords**: : Response Surface Methodology (RSM), optimization, Machine learning modelling,Cassia Fistula

Biodiesel production is very crucial for reducing dependence on fossil fuels, mitigating greenhouse gas emissions, and promoting sustainable energy solutions globally. It offers a renewable alternative that can contribute to energy security and environmental sustainability.This paper presents a machine learning-driven optimization framework using Response Surface methodology(RSM) for enhancing Cassia Fistula based biodiesel production efficiency and reducing carbon monoxide(CO) emissions.It also focuses on comparative study and practical experimentation on the effect of various nozzle holes with biodiesel fuel blends like B20,B100,Diesel,B5,Cassia Fistula biodiesel and obtaining the engine performance including various efficiency metrics.It also aims to do a predictive modelling of CO emissions from biodiesel combustion using various machine learning algorithms. Techniques including Multiple linear regression,Support Vector regression,KNN regressor, decision tree regressor,random forest regressor and ensemble methods like various Bagging and boosting techniques like Xgboost Regressor,Lightgbm Regressor,Catboost regressor and deep learning techniques like Neural networks are applied to develop accurate models based on comprehensive datasets of biodiesel properties and combustion conditions.

## References

[1] Manzoore Elahi M. Soudagar , Sagar Shelare , Deepali Marghade , Pramod Belkhode, Mohammad Nur-E-Alam ,Tiong S. Kiong ,S. Ramesh,Armin Rajabi,Harish Venu,T.M. Yunus Khan,MA Mujtaba,Kiran Shahapurkar a,MA Kalam,I.M.R. Fattah. Optimizing IC engine efficiency: A comprehensive review on biodiesel, nanofluid, and the role of artificial intelligence and machine

[2] Ka In Wong, Pak Kin Wong , Chun Shun Cheung , Chi Man Vong .Modeling and optimization of biodiesel engine performance using Advanced machine learning method

[3] James Pullen, Khizer Saeed. Factors affecting biodiesel engine performance and exhaust emissions.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Investigations of mineral wool type insulations on Improved Biomass Cookstove

**KINNARI MODI[1], DARSHIT S UPADHYAY[1], AMITA CHAUDHARY[1], NIRAJ SHAH[1]***
[1]Institute of Technology, Nirma University, Ahmedabad, Gujarat, India
*Corresponding author: e-mail: niraj.shah@nirmauni.ac.in

**Keywords**: insulation, improved biomass cookstove, economic thickness of insulation, thermal analysis, emissions studies, economic analysis

The present investigations are related to improved thermal performance and reduced emissions due to using three mineral wool types of insulations with two different thicknesses applied to the Improved Biomass Cookstove (IBC) and Heat Box (HB). HB is used as a heat recovery unit. Based on surface temperature without insulation and literature it is decided that wool insulation is best suited for such applications. Thus, the insulations used are rock wool, glass wool, and cera wool. Based on the economic thickness of the insulation study and the available thickness of insulation in the market, 25 and 50 mm thick insulation is applied on IBC and HB. The teak wood is used as the feedstock. Experiments were conducted as per the Bureau of Indian Standards (BIS) testing protocol. Thermal studies cover energy and exergy efficiency, burning rate, firepower, useful firepower, and specific fuel consumption. Emissions investigations measure the particulate matter and emission gases released while using IBC. The study reveals that the use of insulation with different thicknesses resulted in an improvement in thermal efficiency by 1% to 3%. It is also observed that the use of insulation reduces emissions and PM. All insulations are of the same family having a little difference in their thermal conductivity however their prices vary so the economic analysis along with performance and emission observations will be used to determine the appropriate insulation material and thickness.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Ionic liquids for energy production

**SUNITA RAJAMANI***

Department of Chemistry, School of Chemical Sciences, St. Joseph's University, Langford Road, Bengaluru 27
*Corresponding author: e-mail: sunita.rajamani@sju.edu.in

**Keywords**: biofuels, batteries, energy storage, ionic liquids

Energy is a modern-day requirement. Energy can be derived from various waste sources like agricultural, animal, food, byproducts of biodiesel. Most of these wastes are untreated and cause harm to the society. There are definitely lot of lab scale approaches using model compounds to satisfy the proof of concept, but a very few represent the crude systems. The objective of this study is to update use of ionic liquids and highlighting its reliability in lab models towards the transition to industrial systems. Most of the energy production from these sources require organic solvents or corrosive acids or bases, and hence this study will target use of ionic liquids (ILs). ILs are polar solvents with good catalytic properties. They have been proven very useful giving easy recyclability in most of the cases. A small section will focus on use of ILs for batteries and supercapacitors. The second objective will be to select aspects of the process to best suit the circular bioeconomy and making it critically feasible in real industries and identifying the challenges.

## References

[1] Rajamani, S., Kolla, S.S.N., Gudivada, R. *et al. Int J Environ Res* **17** (2023).
[2] K.J. Jisha, S. Rajamani, D. Singh, G. Sharma, RL Gardas, *J Ionic Liq*, **2** (2022) 100037.
[3] Rajamani, S., Santhosh, R., Raghunath, R. *et al.* Value-added chemicals from sugarcane bagasse using ionic liquids. *Chem. Pap.* **75 (**2021).
[4] S Rana, RC Thakur, HS Dosanjh, Solid State Ionics, **400** (2023), 116340.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# A Comprehensive Review on the Optimization of Emulsified Biodiesel-Fueled Engines Using AI and ML Techniques

NAGESH BABU VEMULA[1], SHAIK FAROOQ[1], RADHA KRISHNA GOPIDESI[2*]

[1]Department of Mechanical Engineering, Vignan's Foundation for Science Technology and Research, Vadlamudi, 522213, India
[2]Department of Mechanical Engineering, Vignan's Lara Institute of Technology & Science, Vadlamudi, 522213, India

*Corresponding author: e-mail: grkvlits@gmail.com

This review comprehensively examines the optimization of emulsified biodiesel-fueled diesel engines using advanced Artificial Intelligence (AI) and Machine Learning (ML) techniques. Emulsified biodiesel, a blend of biodiesel and water, offers significant potential for enhancing engine performance and reducing emissions, but its inherent variability necessitates sophisticated optimization methods. The integration of AI and ML techniques, including Artificial Neural Networks (ANNs), Genetic Algorithms (GAs), Support Vector Machines (SVMs), and hybrid methods, provides robust solutions for improving engine performance, optimizing emissions, and refining combustion characteristics. This review explores the applications of these techniques in predictive modeling, real-time optimization, emission prediction, and combustion control, highlighting successful case studies. By leveraging these advanced technologies, emulsified biodiesel-fueled engines can achieve superior efficiency, reduced environmental impact, and optimized operational parameters, paving the way for sustainable and efficient energy solutions.

**Keywords**: Emulsified Biodiesel, Artificial Intelligence, Machine Learning, Optimization, Emission, Combustion

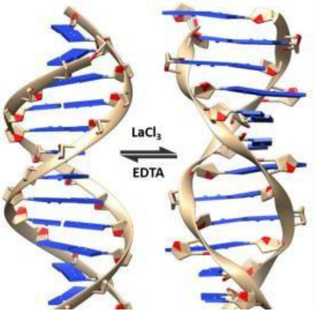
# Lanthanide-induced left-handed DNA: A biophysical and thermodynamics study

**PARTHA S. NIAL[1,2], UMAKANTA SUBUDHI[1,2,*]**

[1]DNA Nanotechnology & Application Laboratory, CSIR-Institute of Minerals & Materials Technology, Bhubaneswar 751 013, Odisha, India
[2]Academy of Scientific & Innovative Research (AcSIR) Ghaziabad 201002, India.
*Corresponding author: e-mail: usubudhi@immt.res.in

**Keywords**: Z-DNA, CD, ITC, Lanthanides, B-Z transition

The typical double stranded DNA is a right-handed helical structure referred to as B-form and considered to be the most stable conformation. Occasionally, this DNA molecule alter their conformation in response to specific situation or external stimuli to form different non-canonical structure such as A-DNA, Z-DNA, Triplex DNA, and G-quadruplex. Among these structures, Z-DNA is found to be most distinct conformational transition with difference in the structural arrangement. In contrast to right-handed B-DNA, the Z-DNA has left-handed orientation. This Z-DNA occurs naturally by means of negative supercoiling or by the induction of positively charged monovalent, divalent and trivalent cations.



The study investigates the impact of lanthanides ($LaCl_3$, $CeCl_3$ and $PrCl_3$) on the conformational transition between the B-form and Z-form of DNA. We employ a combination of biophysical techniques, including Circular dichroism, Isothermal titration calorimetry, Fourier transform infrared, Zeta potential and Molecular dynamics simulations to elucidate the mechanism of B-Z transition. Our results reveal a lanthanide-dependent modulation of the DNA helical structure, leading to the conversion from the canonical B-DNA to the left-handed Z-DNA in $(CG)_n$ repeat and condensation in $(GC)_n$ repeat. Altered helical parameters, base pair stacking and overall DNA geometry upon lanthanide binding has been characterized using spectroscopic analysis. The decrease in Gibbs free energy during ITC indicates a spontaneous reaction and provides the specific binding sites and coordination geometry of lanthanide ions within the DNA double helix. Molecular dynamics simulation further complements our experimental findings, offering a dynamic perspective on the temporal evolution of the B-Z transition process. We observe that lanthanides play a crucial role in stabilizing the Z-DNA conformation in $(CG)_n$ repeat, providing a foundation for understanding the thermodynamics and kinetics of B-Z transition.

## References

[1] P.S. Nial, **U. Subudhi***. **Int. J. Biol. Macromol.** 266, 131238, **2024**.
[2] P.S. Nial, C. Sathyaseelan, M.M. Bhanjadeo, K.D. Tulsiyan, T. Rathinavelan, **U. Subudhi**. **J. Mol. Liq.** 407, 125173 **2024**
[3] M.M. Bhanjadeo, P.S. Nial, C. Sathyaseelan, A.K. Singh, J. Dutta, T. Rathinavelan, **U. Subudhi***. **Int. J. Biol. Macromol.** **2022**.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermal properties analysis of silk fibroin biomaterial film prepared from *Antheraea frithi* Moore cocoon for potential biomaterial applications

**Sanasam Yaiphabi[1,2], Senjam Sunil Singh[2], Raghumani S. Ningthoujam*[1], and S Kunjeshwori Devi*[2]**
[1]Chemistry Division, Bhabha Atomic Research Centre, Mumbai, India – 400085
[2]Department of Biochemistry, Manipur University, Canchipur, Imphal, Manipur, India – 795003
To whom correspondence should be addressed:
*Email: rsn@barc.gov.in kdsanjenbam@yahoo.com

**Keywords**: Silk fibroin films, biomaterials, differential scanning calorimetry (DSC), thermogravimetric analysis (TGA)

## Abstract:

Silk fibroin served as a versatile biomaterial for fabrication of films, hydrogels and scaffolds for various biomedical applications by virtue of its excellent biocompatibility, mechanical strength and thermal properties. In the present study, regenerated silk fibroin solution from the cocoons of *Antheraea frithi* Moore was used to prepared the silk fibroin films. The thermal properties of the silk fibroin films were characterized by differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). From the thermal properties analysis results, it was confirmed that silk fibroin films are more thermally stable than the domesticated silks in nature. Therefore, the thermal properties study will allow the utilization of silk fibroin biomaterial film from the cocoon shell of *Antheraea frithi for* various biomedical applications.

### References

[1] Kweon H, Um I, and Park YJP. Thermal behavior of regenerated Antheraea pernyi silk fibroin film treated with aqueous methanol. 2000;41:7361-7.

[2] Tsukada M, Freddi G, Gotoh Y, and Kasai NJJoPSPBPP. Physical and chemical properties of tussah silk fibroin films. 1994;32:1407-12.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Effects of biogenic nanoadditives on diesel engine combustion, performance and emission characteristics

**SHALU YADAV[1]*, AJIT K. PRAJAPATI[2], ABHAY K. CHOUBEY[1], RAKESH KUMAR[2]**

[1] Dept. of Sciences and Humanities, Rajiv Gandhi Institute of Petroleum Technology Jais, Amethi, Uttar Pradesh – 229304, India
[2] Dept. of Chemical and Biochemical Engineering, Rajiv Gandhi Institute of Petroleum Technology Jais, Amethi, Uttar Pradesh – 229304, India
*Corresponding author: e-mail: 20bs0009@rgipt.ac.in

**Keywords**: biogenic nanoadditives, metal oxides, blending, emissions

The demand for efficient and low emission fuels for diesel engines are rapidly increasing. Therefore, numerous experts worldwide are focused on developing fuels to enhance the efficiency and mitigating emissions from diesel engines. The incorporation of biogenically synthesized nanoadditives to fuels has garnered attention among the multiple approaches established in recent years. Reportedly, nanoparticles have been found to enhance the modified diesel fuel's combustion, performance and emission properties, leading to an overall improvement in the performance of diesel engines and a notable decrease in engine emissions. One of the best additives for lowering emissions from diesel engines is biogenic nanometal oxide synthesized from plant extracts. They can drastically cut fuel consumption and pollution from diesel engines. $CeO_2$, $MgO_2$, $MnO_2$, $Al_2O_3$, $CoO_2$, $ZnO_2$, $TiO_2$, $CuO_2$, $ZrO_2$, are a number of metal oxide based nanoadditives reported recently. Other nanomaterials such as CNTs, graphite oxide, graphene oxide, biochar etc. are also being reported concurrently. In this work we put forward a detail discussion on the recent advancements, challenges and future perspectives of nanoadditives fuels, including their potential as reactive additives with diesel and biodiesel mixes for use in diesel engines, as well as their performance, combustion, and emission characteristics.

### References

[1] A. E. Atabani, et al. A comprehensive review on biodiesel as an alternative energy resource and its characteristics. *Renew. Sustain. Energy Rev*. **2012**, *16*, 2070–2093.
[2] S. Tamrat, V.R. Ancha, et al. Emission and performance analysis of diesel engine running with $CeO_2$ nanoparticle additive blended into castor oil biodiesel as a substitute fuel. *Sci Rep* **2024**, *14*, 7634.
[3] S. Vellaiyan, Enhancement in combustion, performance, and emission characteristics of a diesel engine fueled with diesel, biodiesel, and its blends by using nanoadditive. *Environ Sci Pollut Res* **2019**, *26*, 9561–9573.
[4] D. B. Munuswamy, Y. Devarajan, S. Ramalingam, S. Subramani, N. B. Munuswamy, Critical Review on Effects of Alcohols and Nanoadditives on Performance and Emission in Low-Temperature Combustion Engines: Advances and Perspectives. *Energy Fuels* **2022**, *36*, 7245– 7268.
[5] P. R. Shah, A. Ganesh, A comparative study on influence of fuel additives with edible and non-edible vegetable oil based on fuel characterization and engine characteristics of diesel engine specific gravity. *Appl. Therm. Eng*. **2016**, *102*, 800-812.

T4- OP 13

# MODELING AND SIMULATION OF A TORREFACTION GAS FILTRATION SYSTEM

**SHIV PRAKASH DADHICH[1,2*], KAMAL KISHORE KHATRI[1,2], MOHIT MAKKAR[1], PRIYANSHU JAIN[1]**

[1] Department of Mechanical & Mechatronics Engineering, LNMIIT Jaipur India (302031)
[2] Centre for Energy and Environment Studies, LNMIIT Jaipur
*Corresponding author: e-mail: 19pmm003@lnmiit.ac.in

Torrefaction process is thermal heat treatment of biomass. Torrefied charcoal is primary product and torrefaction gas (alternative fuel) and tar are secondary product of torrefaction process. Torrefaction gas is used as a heating source in torrefaction process after purification process i.e. removal of tar content. Tar content are hydrocarbons, which removes from torrefaction gas with proper quenching methods. In this work a heat exchanger was modeled and simulated on ANSYS Fluent with optimum controlled conditions i.e. temperature, residence time, mass flow rate of gas. A controller was designed to maintain dew point temperature of process for minimization of residence time and maximization of tar removal from torrefaction gas. Optimum residence time was 1.5 min. for water cooled indirect contact heat exchanger and mass flow rate of torrefaction gas is 2.5 kg per hour for smooth process. Torrefaction gas temperature reduces to tar dew point temperature in proposed heat exchanger of process. Overall system controlled by PID controller with steady state error 0.01 and steady state time 30 seconds. Proposed system significantly improves quality of torrefaction gas with minimum resources of energy.

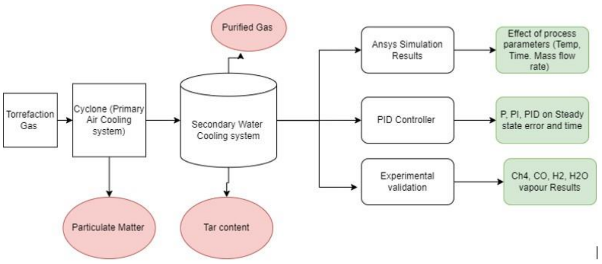


Figure No. 1: Graphical Abstract

## References

[1] J. Shankar Tumuluru, S.Sokhansanj, J. Richard Hess, C. T. Wright, and R. D. Boardman *Energy Reports*, 5 (**2019**) 909-918.

[2] P.V. Gopi Krishna Rao, M. V. Subramanyam, and K. Satyaprasad, *Journal of Control & Instrumentation*, 4(1) (**2012**) 16-22

[3] M. Lee, M. Shamsuzzoha, and T.N. Luan Vu, ―IMC-PID Approach: An Effective way to get an Analytical Design of Robust PID Controller, International Conference on Control, Automation and Systems, Seoul, Korea, pp. 2861–2866, **2008**.

# Lattice Boltzmann Method comparison for the microneedles and hollow micro needles assisting TDD model

**SPURTHI JOANNA SELLADURAI[1], NEETU SRIVASTAVA[2]*,**

[1] Department Of Mathematics, Amrita Vishwa Vidyapeetham, Bengaluru , India
[2] Department Of Mathematics, Amrita Vishwa Vidyapeetham, Bengaluru , India

*Corresponding author: e-mail*:* s_neetu@blr.amrita.edu

**Keywords**: Transdermal drug delivery, microneedles, Lattice Boltzmann Method

In this paper we have studied to estimate the appropriate drug dosage for each patient, which is important to prevent overdosing or ineffectiveness, using Lattice Boltzmann Method (LBM). Another approach for transdermal drug delivery (TDD) is through microneedles via skin in order to bypass the stratum corneum which acts as the primary barrier to deliver drug via skin. The most common transport phenomenon in TDD systems is known to be diffusion. Hence, in relation with diffusion, we studied the effects of diffusion coefficient, drug concentration and length of the needle in the TDD system to treat the diseased person using LBM. Fick’s second law has been used to model the drug's transdermal movement. Conclusions on flux and cumulative flux of the drug has been made.

**References**

[1] Madhihah, S., et al. "Analytic solution for hollow microneedles assisted transdermal drug delivery model." *Int. J. Appl. Eng. Res* 13.1 (2018): 737-742.
[2] Benslimane, Abdelhakim, et al. "Mathematical modeling of transdermal drug delivery using microneedle." *Materials Today: Proceedings* 53 (2022): 213-217.
[3] Safdari, Arman, and Kyung Chun Kim. "Lattice Boltzmann model of percutaneous drug absorption. ." *Theoretical and Applied Mechanics Letters* 9.1 (2019): 1-6.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Isolation of Protease Enzyme from Fish Visceral Wastes and its Application in Leather Processing

**UMAMAGESHWARI. RAJKUMAR[1]*, JAYANTHI. DURGA[2]**

[1,2] Department of Chemical Engineering,
Sri Sivasubramaniya Nadar College of Engineering, Affiliated to Anna University, Kalavakkam,
Tamil Nadu 603110, India.
*Corresponding author: e-mail: umamageshwari2350561@ssn.edu.in

**Keywords**: enzymatic dehairing, protease enzyme, environmental hazards, leather manufacturing

The leather manufacturing process can be broadly classified into three main processes: Pre-tanning, Tanning and Post-tanning. Pre-tanning procedure primarily comprises of Soaking, Liming, Deliming, Batting and Pickling. The common chemical used in liming for hair removal is the adoption of sulphide which customises the conventional method of dehairing. But enzymes are an eco-friendly substitute for the conventional lime- sulphide dehairing process. In this research, the protease enzyme was segregated from fish visceral wastes. The specific protease activity is 12.128 U. Enhanced protease activity of the segregated protease enzyme in crude form was found at a pH of 9.0 and at a temperature of 37℃. Further, the raw protease enzyme was tested for its dehairing competence of goat skins. Thorough removal of hair from the goat skin was found with the enzyme treated. The physical characteristics which include tensile strength, tear strength, elongation, grain crack, water vapour permeability and colour fastness to rubbing of enzymatic wet blue has shown better results. The SEM and histology analysis were performed and the surface and cross-section of the crust leathers were monitored. The major necessity for replacing enzymes in the place of lime/ sulphide is that enzyme aided process reduces the environmental hazards. The pollution loads which were observed in terms of Biological Oxygen Demand (BOD), Chemical Oxygen Demand (COD) and Total Dissolved Solids (TDS) showed a significant reduction in the enzymatic dehairing waste stream when compared to conventional dehairing waste stream.

## References

[1] N. R. Kamini, C. Hemachander, J. Geraldine Sandana Mala and R. Puvanakrishnan, Microbial enzyme technology as an alternative to conventional chemicals in leather Industry, *Current Science*, 1999, 77(1), 80-86.

[2] R. Saranya, J. Jayapriya, A. Tamil Selvi, Purification, characterization, molecular modeling and docking study of fish waste protease, *Int. J. Biol. Macromol*, 2018, 118, 569- 583.

[3] Jayanthi Durga, Ramakrishnan Ramesh, Chellan Rose, Chellappa Muralidharan, Role of carbohydrases in minimizing use of harmful substances: leather as a case study, *Clean Technologies and Environmental Policy*, 2017, 18,1–9.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

---

# The state of the art of the development of Zinc based biodegradable materials- A brief review

**MR.K.KAMALAKANNAN[1]*, DR.K.GANESABALAMURUGAN[2], DR.M.VINOTH[3]**

[1]Senior Assistant Professor, IFET College of Engineering,Villupuram-605108,Tamilnadu,India
[2] Assistant Professor, IFET College of Engineering,Villupuram-605108,Tamilnadu,India
[3]Assistant Professor, IFET College of Engineering,Villupuram-605108,Tamilnadu,India
*Corresponding author: e-mail: kamalakannanat@gmail.com

**Keywords**: Biodegradable materials, Zinc, Biomedical implants

Zinc-based biodegradable materials are gaining significant attention as potential candidates for next-generation biomedical implants, offering a promising alternative to conventional materials such as magnesium and iron.

Zinc plays a vital role in various physiological processes, including cell proliferation, enzyme function, and bone metabolism. It is an essential trace element that supports the growth and development of new cells, which is crucial for the integration and functionality of biomedical implants. The release of Zn2+ ions during the degradation process is beneficial as it can suppress the proliferation of smooth muscle cells, reducing the risk of restenosis in cardiovascular applications, while simultaneously promoting osteogenesis in orthopaedic applications.

Zinc-based biodegradable materials offer several advantages over magnesium and iron, including a more suitable degradation rate and favourable biological interactions. However, the main limitation remains the enhancement of pure zinc’s mechanical properties to meet the demands of medical applications. On-going research focuses on optimizing alloy compositions and processing techniques to address these challenges.

This review examines the latest developments in Zn-based BMs, highlighting their benefits and drawbacks compared to other BMs. It also explores how alloy composition, microstructure, and processing techniques influence the mechanical and corrosion properties of Zn-based BMs.

**T4- OP 17**

# Crystallization kinetics to achieve Stoichiometric Combeite ($Na_2Ca_2Si_3O_9$) and Silicorhenanite ($\beta$-$Na_2Ca_4(PO_4)_2SiO_2$) Single Phasic Bioactive Glass System

**VIJAYAKUMARI.S, BALAKUMAR.S***

National Centre for Nanoscience and Nanotechnology, University of Madras, Chennai – 600025, India
*Corresponding author: e-mail: balasuga@yahoo.com

**Keywords**: thermal analysis, TG-DTA, kinetic models, activation energy.

The great versatility and suitability of bioactive glass in the field of medicine led to the advancement of many clinical products for the well-being and rehabilitation of patients. One of the major drawbacks focused in this study is the crystallization of the bioactive glasses. The crystallization or partial crystallization of the bioactive glasses is reported to decrease the bioactivity of the material at an increasing temperature during heat treatment. The reports show that low-temperature sintering of silicate glasses results in a sodium-rich phase whereas higher-temperature sintering yields a phosphate-rich phase[1,2].

Combeite ($Na_2Ca_2Si_3O_9$), a silica-rich crystallographic phase, and Silicorhenanite ($Na_2Ca_4(PO_4)_2SiO_4$), a phosphate-rich crystallographic phase form during heat treatment of bioactive glass compositions and play a major part in deciding the properties of the biomaterials. Determining crystallization kinetics is one of the appreciable routes to achieve the desired phase and predict the bioactivity of the material. From the study, it is found that sol-gel derived bioactive glasses require 141.49 kJ/mol to form the Combeite phase and only 81.95 kJ/mol of activation energy to form the Silicorhenanite phase. The obtained results are lower than the energy required for crystalline hydroxyapatite and offer a unique material for rapid bioactivity.

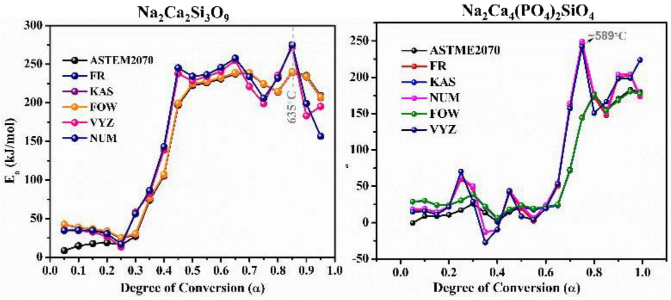


Fig. 1 : α Vs $E_a$ curve of (a) Combeite - $Na_2Ca_2Si_3O_9$ and (b) Silicorhenanite - $Na_2Ca_4(PO_4)_2SiO_4$ crystallographic phases

## References

1 M. Magallanes-Perdomo, S. Meille, J.-M. Chenal, E. Pacard and J. Chevalier, *Journal of the European Ceramic Society*, 2012, **32**, 2765–2775.

2 L. Lefebvre, J. Chevalier, L. Gremillard, R. Zenati, G. Thollet, D. Bernache-Assolant and A. Govin, *Acta Materialia*, 2007, **55**, 3305–3313.

**T5- OP 01**

# Thermal denaturation and aggregation of horn keratin observed by differential scanning calorimetry (DSC)

**F. Gimeno[1]*, G. Vaca-Medina[1], A. Rouilly[1]**

[1]Laboratoire de Chimie Agro-Industrielle (LCA), Université de Toulouse, INRAE, Toulouse INP,
31030 Toulouse, France

**Keywords**: thermal analysis, DSC, protein denaturation, protein aggregation

The hierarchical structure of keratin has been extensively studied but there is no clear explanation regarding the mechanism of denaturation of this protein. This is however an essential step towards a better understanding of the transformations taking place during the new molding processes which aim to valorise this biopolymer[1].

The aim of this work was to study the possibility of observing structural changes (denaturation) of horn keratin by DSC and evaluating the influence of sample mass, heating rate, water content in the system and the thermal conductivity of the media. The addition of silicon oil to horn keratin improved the thermal conductivity of the media leading to a better understanding of protein denaturation. Similarly, the moisture content greatly influences the keratin denaturation, allowing a greater enthalpy of denaturation and a shift of the phenomena to the lower temperatures[2].

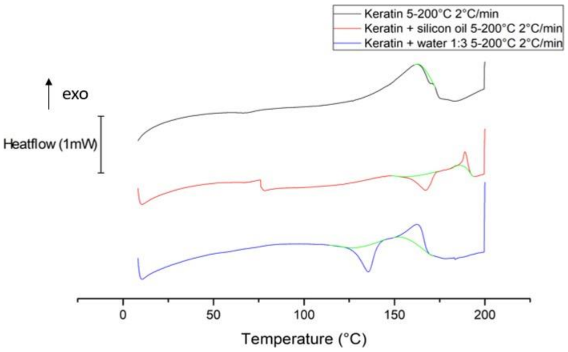


Fig. 1 : DSC curves of horn keratin with different thermal conductor and a heating rate of 2°C/min

Analysis with lower heating rates with addition of a thermal conductor lead to the observation of an exothermic peak associated to keratin aggregation right after its denaturation, highlighting a kinetic aspect to this structural modification [Fig. 1].

**References**

[1]M. Jumeaux, F. Touchaleaume, V. Durrieu, V. Vandenbossche, G. Vaca-Medina, et A. Rouilly, *ACS Sustainable Chem. Eng.*, vol. 11, nº 42, p. 15423-15431, oct. 2023.

[2]A. Rouilly, O. Orliac, F. Silvestre, et L. Rigal, *Thermochimica Acta*, vol. 398, nº 1, p. 195-201, mars 2003.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Precision in Laser Cutting of KFRP Composites: Insights from Taguchi and ANN Based Tech niques in Materials Engineering

**ASHISH A.DESAI [1,2] , S.N. KHAN[1]**

[1]Mechanical Engineering Department, Rajarshi Shahu College of Engineering, Tathawade, Pune, Maharashtra, India
[2] Automation and Robotics Department, Sharad Institute of Technology College of Engineering, Yadrav, Maharashtra, India
*Corresponding author: e-mail: ashishdesai@sitcoe.org.in

**Keywords**: Kevlar Fiber Reinforced Plastic, Laser Cutting, Optimization, Taguchi Method, Artificial Neural Networks, Process Parameters, Efficiency, Surface Quality

Laser machining of Kevlar fiber reinforced polymer (KFRP) composites aims to improve surface accuracy and quality by adjusting process factors such as laser type and power, feed rate, and cutting speed. This work uses the Taguchi approach to methodically organize experiments and investigate the effects of key elements such as laser power, cutting speed, pulse frequency and assisted gas pressure. The L9 orthogonal array is used to efficiently search the parameter space to find the best settings to minimize cut width and surface roughness. To improve the optimization process, an artificial neural network (ANN) model is created and trained on experimental data.

The ANN model provides a powerful tool for predicting the results of different parameter combinations and fine-tuning the laser cutting process, which ensures the accuracy and excellent surface quality of KFRP composites. By integrating Taguchi and ANN methods, laser cutting dynamics significantly improves cutting quality and process efficiency. Experimental results show that parameter optimization can significantly improve laser cutting accuracy and achieve narrower widths and smoother surfaces. This combined approach provides a robust framework for optimizing the laser cutting process of KFRP composites advanced manufacturing and paves the way for ad applications with high demands on precision and quality. This finding highlights the potential of hybrid optimization techniques in advancing the processing of composite materials and provides valuable insights into the field of laser processing. The ANN predicted values were very close to the experimentally measured values for Ra and Kwf with an accuracy of 93.05% and 86.13%. So ANN can be safely applied for prediction of VB and Ra in current manufacturing industry so that product quality can be improved. Then, the effect of machining parameters was calculated for Ra and Kwf by signal to noise (S/N) ratio and analysis of variance (ANOVA). From the calculation of S/N ratio, it was found that spindle speed has the greatest influence on Ra and Kwf

which is succeeded by feed rate and depth of cut. The ANOVA calculation also validates the findings of the S/N ratio calculation for VB and Ra. Cutting in the right dimension combination will help reduce Ra Kwf and improve product quality.

The findings emphasize the potential of hybrid optimization strategies in enhancing composite material processing and provides important insights into the area of laser processing. The ANN projected values for Ra and Kwf were quite close to the experimentally measured values, with 93.05% and 86.13%, respectively. As a result, ANN can be properly utilized for forecasting VB and Ra in today's manufacturing industry, allowing for enhanced product quality. The influence of machining settings on Ra and Kwf was then calculated using the signal-to-noise (S/N) ratio and ANOVA.

T5- OP 03

# Structural and Thermal Behaviours of Iron-based Gas Atomized Powders

**Rajat K. Roy*, Premkumar M., K. Gopala Krishna, Ashis K. Panda**

[1]CSIR-National Metallurgical Laboratory, Jamshedpur-831007, India

*Corresponding author: e-mail: rajat@nmlindia.org

**Keywords**: Gas atomization, Amorphous, Powders, DSC.

Iron based amorphous alloys (FeBSiCP) have wide applications owing to its high strength and wear resistance, good corrosion resistance, ultra-soft magnetic properties and low material cost [1]. These alloys are generally processed as thin foils in micron range thickness and unable to make bulk form. However, the alloys can be processed as fine powders by gas atomizer (GA), and subsequently manufactured as bulk components by 3-D printing technique with utilization of GA powders [2].

The present investigation is focused on the development of FeBSiCPCrMo amorphous alloy powders by a gas atomizer. The powders were obtained with 0-300 micron size range, varying their thermal and structural behaviours as a function of particle size. DSC thermograms of all powder size explain same points on the endothermic change (Fig.1) of glass transition temperature (Tg~474°C), and followed by an exothermic peak of crystallization, associating with crystallization onset (Tx~527°C) and peak (Tp~532°C) temperatures. However, thermal enthalpy ($\Delta H$) of powder decreases with increasing powder diameter, justifying the increase of crystallinity with powder size. It is also justified by XRD patterns, indicating powder crystallinity above 63 micron size.

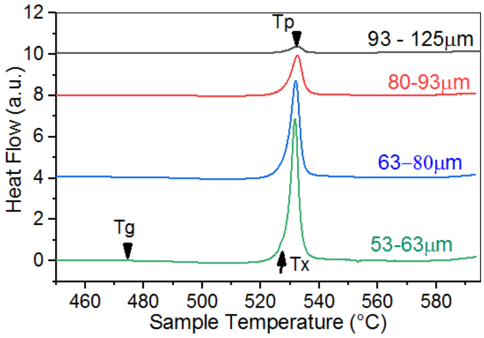


Fig. 1 : DSC thermograms of different size range gas atomized powders, indicating glass transition (Tg), crystallization onset (Tx) and peak crystallization (Tp) temperatures.

## References

[1] J.M. Park, J.H. Na, D.H. Kim, K.B. Kim, et al., Phil. Mag., 90 **(2010)** 2619-2633.
[2] V. V. Popov, M. L. Grilli, A. Koptyug, L. Jaworska, et al., Materials, 14 **(2021)** 909.

# Thermal Analysis and Characterization of Natural Cellulosic Fiber from *Azadirachta Indica* and its Polymer Composites

**JITENDER YADAV[1], PL RAMKUMAR[*1], AJIT KUMAR PARWANI[1]**

[1] Institute of Infrastructure, Technology, Research and Management, Ahmedabad-380026, India
*Corresponding author: e-mail: plramkumarno1@gmail.com

**Keywords**: Thermal analysis, DSC, TGA, Wood polymer composites

This research investigated the thermal and rheological properties of wood polymer composites (WPCs) incorporating natural fibers derived from *Azadirachta Indica* (AI or neem tree). Comprehensive characterization of AI wood dust revealed a high cellulose content of 70.36 wt%, low lignin content of 13.2 wt%, minimal wax content of 0.38%, and a crystallinity index of 65.62%. Thermal analysis of pure AI wood showed enhanced thermal resistance, with a peak at 346.6°C in the derivative thermogravimetric (DTG) curve. The study on WPCs with varying AI wood fiber compositions demonstrated a reduction in melt flow index from 4.4 to 1.45 g/10 min as wood content increased, indicating reduced flowability. Differential scanning calorimetry (DSC) (Table 1) and thermogravimetric analysis (TGA) (Figure 1) revealed an increase in the decomposition temperature of WPCs with increasing wood content, suggesting improved thermal stability. The composite with 12 wt% wood content exhibited a maximum crystallinity index of 62.59%. The comprehensive analysis of AI wood dust and its polymer composites highlights their potential for developing environmentally friendly composites for various applications.

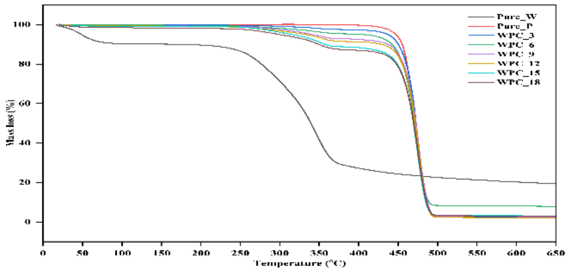


Figure 1: TGA analysis of WPC’s

Table 1: Characterization data of WPC's composites determined through DSC.

| Sample | Crystallization range of WPC | | Enthalpy of crystallization of WPC | Melting peak of WPC | Enthalpy of melting of WPC |
|---|---|---|---|---|---|
| | $T_{onset,c}$ (ºC) | $T_c$, (ºC) | $\Delta H_c$ (J/g) | $T_m$, (ºC) | $\Delta H_m$ (J/g) |
| LLDPE | 109.9 | 107.5 | 143.71 | 122.71 | 174.22 |
| WPC_3 | 110.82 | 108.1 | 131.86 | 122.52 | 157.39 |
| WPC_6 | 110.87 | 108.6 | 134.74 | 122.75 | 157.02 |
| WPC_9 | 111.05 | 108.7 | 133.71 | 122.74 | 160.29 |
| WPC_12 | 111.06 | 109 | 130.34 | 122.69 | 161.38 |
| WPC_15 | 111.21 | 108.7 | 143.69 | 122.31 | 141.68 |
| WPC_18 | 111.02 | 108.1 | 118.18 | 122.26 | 125.95 |

# Investigation on possible use of Aloe Vera or mixed Aloe Vera hydrogels with gelatin or HPC as Iodophors and the controlled release of Iodine from the hydrogels

**M. ASHARANI DEVI AND HOMENDRA NAOREM**
Department of chemistry Manipur University, Canchipur, Imphal-795003, Manipur, India
*Corresponding author: e-mail: asharanidevimaisnam@gmail.com

**Keywords**: Aloe Vera, Gelatin, Hydroxypropyl cellulose (HPC), Iodine, Iodophor

Aloe vera gel which contains about 98% water is a natural hydrogel with many health benefit attributes. The present study explores the possibility of employing aloe vera or mixed aloe vera gelatin or HPC gels as template for the entrapment of iodine and their controlled release. Aloe vera gels interact weakly with iodine with no significant shift in the 350 nm triiodide band while significant red shift was observed with gelatin or HPC gels. It was observed that aloe vera gel can entrap about 12% of the available iodine in about 2 h. But when immersed in water, about half the iodine entrapped in aloe vera gel was released in less than 3h indicating that aloe vera gel alone is unlikely to be a good iodophor. On the other hand, gelatin (15%) or HPC (6%) gels can entrap about 64% or 20% iodine in about 13 or 23 h respectively. With a view to improving the iodine entrapment ability with slow and sustained release of the entrapped iodine, mixed aloe vera gels with gelatin or HPC were prepared and tested for their iodine entrapment ability and their release kinetics. Both the entrapment and the release of iodine was monitored the characteristic triiodide band at 350 nm spectrophotometrically.

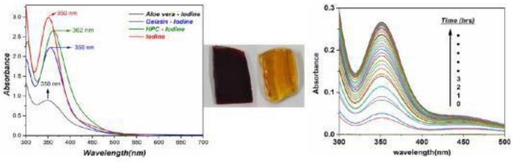


Fig. 1 : UV-Visible spectra of Aloe vera, Gelatin, HPC in presence of Iodine/Iodide solution and spectra of Iodine released in aqueous media

The iodine entrapment ability of aloe vera gel can be increased from 12% to more than 40% by blending aloe vera with gelatin in 1:1 ratio while the time of release is increased from 3 to more than 9 h. While the entrapment ability of the aloe vera gels was not much affected by blending with HPC gels, it was observed the release of the iodine was found to be slow and steady extending to more than 24h. The release of the entrapped iodine followed first order kinetics and the rate constant was found to be higher in case of pure aloe vera gels as compared to the mixed gels. The AFM or SEM profile of the gels showed sharp decrease in the roughness of the aloe vera gels with the entrapment of iodine and also when blended with gelatin.

**References**

[1] H. Naorem, N. S. Singh, Journal of Physical Chemistry B, 111(16), 2007, 4098-4102
[2] H. Naorem, S. D. Devi, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 101, 2013, 67-73
[3] P.L. Bigliardi, S.A.L. Alsagoff, H.Y.E.Kafrawi, J.K.Pyon, C.T.C. Wa, M.A. Villa, International

**T5- OP 06**

# Study on the use of Aloe Vera gel, Gelatin, or their co-gels as templates for entrapment of $Pb^{2+}$, $Cu^{2+}$, or $Fe^{2+}$ from their aqueous solutions

**<u>SORODHONI POTSHANGBAM</u> AND HOMENDRA NAOREM***

Department of Chemistry, Manipur University, Canchipur, 795003, Imphal, Manipur, India
*Corresponding author: e-mail: soropotshangbam@gmail.com

**Keywords**: Hydrogels, Langmuir, Dispersing, sorbate concentration, adsorbent dose

The present study is an attempt to examine if the aloe vera or mixed aloe vera gels with gelatin can be effectively used for the removal of some heavy metal ions like $Pb^{2+}$, $Cu^{2+}$, or $Fe^{2+}$ from their aqueous solution by entrapping them in the gels. Aloe Vera gels were prepared after extracting them from the leaves of aloe vera plants grown in the locality. The mixed aloe vera and gelatin gels were prepared by blending them in definite proportions. The gels or the mixed gels were characterized using FTIR, SEM, EDAX, etc. The gel or the mixed gels were immersed in aqueous solutions containing known amounts of $Pb^{2+}$, $Cu^{2+}$, or $Fe^{2+}$, and the concentration of the metal ion in the solution was monitored as a function of time until it began to saturate. The amount of $Pb^{2+}$ or $Cu^{2+}$ ions entrapped in the gels was determined spectrophotometrically.

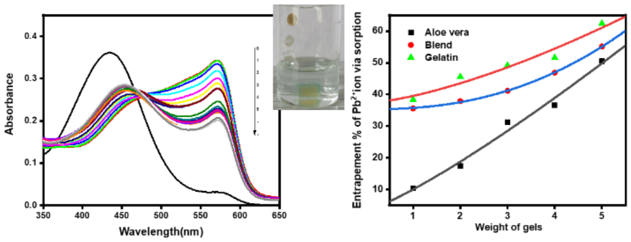


Fig. 1: A UV-Vis spectrum of ligand and Pb-complex after absorption of metal ion by the gel and entrapment % of metal ion by different gel is shown in the graph

It was observed that the entrapment of $Pb^{2+}$ or $Fe^{2+}$, $Cu^{2+}$ions followed the Langmuir isotherm indicating that the entrapment process began with adsorption of the metal ions. The results showed that pure aloe vera gels (about 2 g) can entrap about 65% $Cu^{+2}$, 34% $Pb^{2+}$ or 15% $Fe^{+2}$ ions respectively in about 12 h indicating that among the three metal ions, aloe vera has higher affinity for the $Cu^{+2}$ ions. While the mixed aloe vera and gelatin gel (1:4) showed about 23% or 26% increase in the amount of $Pb^{+2}$ or $Fe^{+2}$ions entrapped by the gels, a sharp decrease to the extent of about 60% was observed in the amount of $Cu^{+2}$ entrapped in the mixed gels. The entrapped metal ions were completely released within 5 h and followed first-order kinetics. The aloe vera and its mixed gels also exhibited good efficiency in regeneration and metal ion recovery. The same gel can be reused without noticeable loss of entrapment capacity for $Pb^{2+}$, $Cu^{2+}$, or $Fe^{2+}$ ions at least up to four repeated 'entrapment-release cycles.

**References**:
[1] D. A, Giannakoudakis, A. Hosseini-Bandegharaei, P. Tsafrakidou et al., *Environ. Manag*, 227 (**2018**) 354-364.

# Investigation on structural properties, thermal stability and photoluminescence properties of biocompatible Eu (III) doped calcium phosphate nanoparticles

**THOUDAM CHANCHAN DEVI [1]*, THIYAM DAVID SINGH [1]**

[1] Department of Chemistry, National Institute of Technology Manipur, Langol 795004, India
*Corresponding author: e-mail: chanchanuniversity@gmail.com

**Keywords**: Calcium phosphate, phase change, luminescent enhancement, biocompatible

Calcium orthophosphates have found numerous potential applications in orthopedic and dental implants and bone tissue engineering due to their highly biocompatible and biodegradable nature of materials. In addition, pH sensitive degradability of calcium phosphate (CaP) nanoparticles (NPs) offers to use as a carriers to transfer therapeutic agents like proteins, drugs, enzymes, nucleic acids, etc.[1] Therefore, due efforts is given on synthesizing different phase and morphology of CaP NPs by various methods for biomedical applications. Herein, CaP NPs doped with $Eu^{3+}$ (3 at %) are synthesized by co-precipitation method with varying pH using ethylene glycol as capping agent as well as solvent media. The as prepared NPs are characterized by XRD, FTIR, FESEM, EDAX, TGA-DSC, etc. The samples synthesized at different pH show formation of different phases of CaP as indicated by XRD. Photoluminescence properties of the synthesized samples are also analyzed and the samples show the peaks related to absorption and emission of $Eu^{3+}$ ions. The emission spectra [Fig. 1] show the variations in the peak intensity with dominant peak at 616 nm corresponding to the electric dipole transition ($^5D_0 \rightarrow {}^7F_2$) of $Eu^{3+}$ ions.[2] MTT assay provides good cytocompatibility of the samples to NIH 3T3 cell line showing promise for their future biomedical use as luminescent nanoprobes.

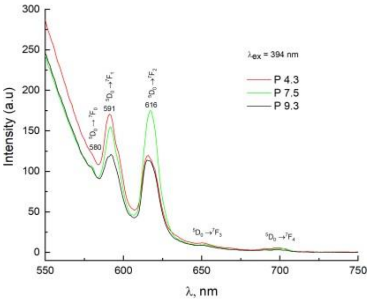


Fig. 1: Photoluminescence emission spectra of as synthesized CaP NPs

**References**
[1] R. Khalifehzadeh, and H. Arami, *Advances in Colloid and Interface Science*, 279 (2020) 102157.
[2] T. Kataoka, S. Samitsu, M. Okuda, D. Kawagoe and M. Tagaya, *ACS Appl. Nano Mater.*, 3 (1) (2020) 241.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

---

# Evaluating the Optimal LLDPE/NaOH-Treated Peanut Shell Powder Blend for Improved Rotational Molding Processability

PRASHANT KHANNA[1]*, PL. RAMKUMAR[2]

[1]Department of Mechanical Engineering, Parul University, Vadodara, Gujarat-391760, India
[2]Department of Mechanical and Aerospace Engineering, Institute of Infrastructure Technology Research and Management, Ahmedabad, Gujarat-380026, India
*Corresponding author: prashantkhanna2003.pk@gmail.com

**Keywords**: Rotational molding, LLDPE, peanut shell, thermal stability

This study explores incorporating NaOH-treated peanut shell powder (TPSP) as a reinforcing filler in linear low-density polyethylene (LLDPE) for rotational molding applications to enhance mechanical and thermal properties [1]. By utilizing the lignocellulosic composition of TPSP, which includes cellulose, hemicelluloses, and lignin, the study investigates its compatibility with LLDPE and potential to improve processability and product performance [2,3]. Tests such as FTIR, particle size analysis, bulk density measurement, melt flow index (MFI), differential scanning calorimetry (DSC), and thermogravimetric analysis (TGA) are conducted to elucidate the behavior of LLDPE-TPSP blends for rotational molding.

FTIR analysis demonstrated the compatibility of blends with 10% to 22% TPSP, emphasizing the need for balanced composition for effective reinforcement. Particle size distribution, bulk density, and MFI analysis confirmed that blends with 10% to 16% TPSP ensured proper flow, packing, and uniform mold filling capability for rotational molding. DSC results showed that blends with 10% to 16% TPSP have increased peak melting temperature and crystallinity, indicating enhanced thermal stability compared to pure LLDPE. TGA supported these findings, showing that a blend with 16% TPSP maintained a processing temperature range comparable to pure LLDPE, with improved thermal stability. Thus, incorporating 16% TPSP was identified as optimal for enhancing rotational moldability, providing improved thermal stability, processability and offering valuable insights for developing bio-based polymer composites for industrial applications.

**References**

[1] Zaaba NF, Ismail H. A Review on Peanut Shell Powder Reinforced Polymer Composites. Polymer-Plastics Technology and Materials. 2019;58(4):349–65.
[2] Oulidi O, Nakkabi A, Boukhlifi F, Fahim M, Lgaz H, Alrashdi AA, Elmoualij N. Peanut shell from agricultural wastes as a sustainable filler for polyamide biocomposites fabrication. J King Saud Univ Sci. 2022;34(6):102148.
[3] Ikladious NE, Shukry N, El-Kalyoubi SF, Asaad JN, Mansour SH, Tawfik SY, Abou-Zeid RE. Eco-friendly composites based on peanut shell powder/unsaturated polyester resin. Proceedings of the Institution of Mechanical Engineers, Part L: Journal of Materials: Design and Applications. 2019;233(5):955–64.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Kinetic Analysis and Pyrolysis Behaviour of Polydimethysilane using Evolved Gas and Thermal methods

**G. SANTHANA KRISHNAN[1]*, A.KEERTHANA[1],**

Materials Science division, CSIR-National Aerospace Laboratories, Bengaluru 560017, India
*Corresponding author: e-mail: keerthana.kjav@gmail.com (Keerthana A),
santhana@nal.res.in (G.S. Krishnan).

**Keywords**: Polydimethylsilane, Pyrolysis, Thermal degradation, kinetics,

## Abstract

Thermal degradation and pyrolysis reactions of Polydimethylsilane (PDMS) were investigated using hyphenated analytical pyrolysis methods viz., evolved gas analyzer with pyrolyzer-gas chromatography/ mass spectrometry and Thermogravimetric analysis(TGA). In this study, qualitative analysis of pyrolyzates evolved during the reactions was obtained by Py-GC/MS. Kinetic results derived through this model free kinetic analysis method using EGA-MS and TGA were compared. The activation energy for the thermal degradation reaction and pyrolysis reaction were found to be in range of 147-192 kJ/mol (mean 170 kJ/mol) & 370-412 kJ/mol (mean 391 kJ/mol) for EGA-MS and 138-189kJ/mol (mean 164 kJ/mol) & 375-404 kJ/mol (mean 389 kJ/mol) for TGA respectively. This suggests that Py-GC/MS can also be used for kinetic analysis of PDMS.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Covalent modification of Cellulose for selective extraction of Mercury ($Hg^{2+}$) and Lead ($Pb^{2+}$)

**DEVANSHU PATHAK[1]*, DOLLY PANCHAL[2], MADHUMITA MUKHERJEE[3], APURBA LAL KONER[4], SUMIT BHAWAL**

[1]Navrachana University, Vadodara-391410, India
[2] Navrachana University, Vadodara-391410, India
Department of Chemistry[3], IISER Bhopal, Bhopal-462030, India
[4] Department of Chemistry, IISER Bhopal, Bhopal-462030, India
*Corresponding author: e-mail: sumitb@nuv.ac.in

**Keywords**: Cellulose, Chelation, ITC, Thermal analysis

This study investigates the removal of Mercury and Lead using microcrystalline cellulose (Hydroxyl value 18.5 mmol/g) modified with selective chelating groups. The associated change in enthalpy on the binding of the metal to the chelating group was investigated through ITC for the corresponding solutions. Cellulose was modified with chelating groups such as EDTA dianhydride, DMSA, and Bismuthiol with the help of amino silane linkers. The synthesized material was characterized by EDAX and FTIR, which indicated covalent modification of cellulose. The efficiency of the covalently linked chelating ligand to bind with Hg and Pb was measured by UV-vis spectrophotometer and complexometric titration respectively. The results showed a 92% and 80% decrease in the concentration of Hg and Pb respectively. The functionalized cellulose powder was also subjected to thermal analysis using DSC and TGA, to indirectly observe any change in material property following functionalization.

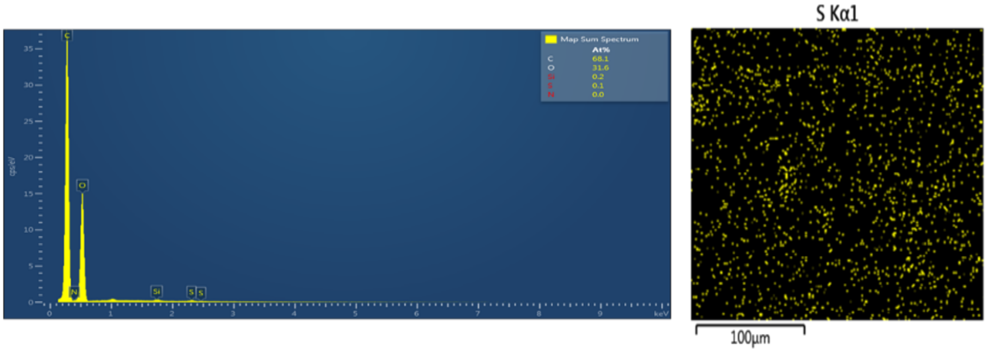


Fig.1: a) EDAX of Bismuthiol modified cellulose based on binding energy
b) Mapping of Sulphur

**References**
[1] Karnitz O, Gurgel L, Gil L, *Carbohydrate Polymers (2010) 79(1) 184-191*
[2] Yoong, A. U., Loo, Y., In *Sains Malaysiana* (2012) (Vol. 41, Issue 2)
[3] Karlsen, V., Heggset, E. B., & Sørlie, M. *Thermochimica Acta*, (2010) *501*(1–2)

---

# Effect of Yttria Concentration on the Mechanical and Thermal Stability of Yttria Stabilized Zirconia (YSZ): First Principles Studies

**MANSINGH YADAV, NABILA TABASSUM, YAMINI SUDHA SISTLA***

Department of Chemical Engineering, Shiv Nadar Institution of Eminence, Delhi NCR, India.
*Corresponding author: e-mail: yamini.sistla@snu.edu.in

**Keywords**: Yttria Stabilized Zirconia (YSZ), Thermal Barrier Coatings, Density Functional Theory, Mechanical properties

Thermal barrier coatings (TBC) are used for high temperature applications such as combustors and gas turbines to protect the base alloy materials from thermal fouling. The TBC assembly consists of a heat-insulating ceramic coating (topcoat) applied over an oxidation-resistant metallic bond coat [1]. A conventional TBC material Yttria-stabilized zirconia (YSZ) in known for its high strength, thermal stability, wear, oxidation and corrosion resistance is widely used as a topcoat for TBC applications [2]. Present study evaluates the effect of concentration of $Y_2O_3$ on the properties of YSZ through First principles calculations. The structural, mechanical, electronic, and thermal properties were evaluated at various mole percent of $Y_2O_3$ in the $(Y_2O_3)_x$ $(ZrO_2)_{1-x}$ matrix where x = 0.11, 0.19, 0.53. From the knowledge of the elastic constants, the mechanical properties (bulk modulus, shear modulus, young's modulus), electronic properties (total and partial density of states), thermal properties (sound velocity, Debye temperature, thermal capacity and minimum thermal conductivity) are numerically estimated in the framework of the Voigt – Reuss – Hill approximation. The results infer that, an increase in mole fraction 'x' of $Y_2O_3$ would lead to an increase in the density (5.48 – 6.0 g/cm$^3$) and hardness (7.35 – 12.72 GPa) of YSZ. Furthermore, the shear modulus of YSZ increased as 84.35 GPa, 99.46 GPa, and 101.37 GPa, for $Y_2O_3$ mole fraction of 11%, 19% and 53% respectively indicating improved rigidity of YSZ. Bulk modulus of $(Y_2O_3)_x$ $(ZrO_2)_{1-x}$ are 178 GPa, 211.16 GPa, and 214 GPa for $Y_2O_3$ mole fraction of 11 %, 19% and 53% respectively suggesting improved deformation resistance of YSZ. Increased young's Modulus as 223.73GPa, 257.88 GPa, 255.73 GPa established that the stiffness of YSZs increases in the order of 11%<19%< 53% of $Y_2O_3$. All the elastic moduli values computed in the present work were within 5% deviation from the reported experimental and computational data [3]. The Cauchy pressure and Pugh's ratio which are indicators of material ductility observed to increase with increase in yittria concentration. The calculated sound velocity, Debye temperature, thermal capacity and minimum thermal conductivity are within 8% deviation from the available experimental and computational results [3]. The anisotropy of $(Y_2O_3)_x$ $(ZrO_2)_{1-x}$ was also evaluated based on the 3-dimensional directional variation of elastic moduli.

References

[1] H. Esmaeilkhanian, F. Sharifianjazi and Elahe, Mater. Today Commun. 37(2023) 107514.

[2] R. Vaben, D. Emil Mack and Mertin Tandler, J. Am. Ceram. Soc.104(2020) 463-471.

[3] Lei Jin, Qinghe Yu and Abdul Rauf, Elastic, Solid State Sci. 14 (2012),106-110.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Assessing the Structural, Mechanical and Thermal Properties of AlCoCrFeNi High Entropy Alloy for High Temperature Applications: Atomistic Simulations

**NABILA TABASSUM, YAMINI SUDHA SISTLA***

Department of Chemical Engineering, Shiv Nadar Institution of Eminence, Delhi NCR, India.
*Corresponding author: e-mail: yamini.sistla@snu.edu.in

**Keywords**: High Entropy Alloys, Thermal Barrier Coatings, Density Functional Theory, Mechanical properties

Turbine blades of aircraft engines are prone to thermo-mechanical damage. Thermal barrier coatings (TBCs) are employed to reduce the temperature induced failure of turbine blades [1]. TCBs are two-layer coatings with ceramic based top coat and metallic alloy-based bond coat. High entropy alloys (HEA) comprising more than five elements have gained attention owing to their remarkable thermal and mechanical stability, oxidation resistance and corrosion and wear resistance. Present study evaluates the effect of aluminum (Al) molar ratio '*x*' on the structural, electronic, mechanical, and thermal properties of aluminium (Al), cobalt (Co), chromium (Cr), iron (Fe) and nickel (Ni) based HEA $Al_xCoCrFeNi$ ($x = 0.0, 0.1, 0.3, 0.5, 0.9, 1.0, 1.5$ and $2.0$) using Density Functional Theory (DFT). Face Centered Cubic (FCC) crystal form of $Al_xCoCrFeNi$ was chosen for $x$= 0.0, 0.1, 0.3, 0.5,1.0 and Body Centered Cubic (BCC) form was chosen for $x$= 0.9, 1.0, 1.5, 2.0 [2,3]. The Special Quasi Random Structure (SQS) models of $Al_xCoCrFeNi$ were used for the property evaluation. Thermodynamic stability criteria and atomic size difference parameters confirm the phase stability of $Al_xCoCrFeNi$ for all molar ratios of Al. Thermodynamic stability of $Al_xCoCrFeNi$ increased with Al molar ratio. Mechanical properties such as elastic moduli, Vickers hardness, fracture toughness, Debye temperature and acoustic wave velocity were computed for a microscopic level strain rate of ±0.7%. The properties computed based on phase change from FCC to BCC at $x$> 1.3 of $Al_xCoCrFeNi$ match well with available experimental and theoretical literature values [2,3]. Elastic moduli, hardness, and fracture toughness decrease with increase in Al concentration. Present study also evaluates the thermo-mechanical stability of the equiatomic AlCoCrFeNi HEA in a temperature range of 298 -2500K. AlCoCrFeNi consists of both FCC and BCC crystal phases. The elastic moduli, hardness, yield stress, and ultimate tensile strength of FCC and BCC AlCoCrFeNi decreased up to 1700K, melting point of the alloy. Just after the melting point 1700 K, all the properties showed a significant drop quantitatively indicating the phase change from solid to liquid of the alloy. This study evidently captures the melting behaviour of the AlCoCrFeNi. Results of present study ascertain that AlCoCrFeNi alloy retains hardness and fracture toughness to significant extent until a temperature of 1500 K, a superior characteristic compared to the conventional turbine blade material Inconel 718.

**References**

[1] S.T. Vagge, S. Ghogare, *Materials Today Proceedings*, 56 **(2022)** 1201.
[2] S. San, Y. Tong, H. Bei et al, *Material Design*, 209 (**2021)** 110071-110084.
[3] M.A.A. Hasan, J. Wang et al. *Journal of Alloys and Compounds, 883* **(2021)**, *160881.*

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermally Stable, Mechanically Robust and Highly Conducting Eutectogels as Electrolytes for Supercapacitors

**OMISH SETHI[1], ASHWANI KUMAR SOOD[1], TEJWANT SINGH KANG[1, *]**

[1]Department of Chemistry, UGC Centre for Advance Studies-II, Guru Nanak Dev University,
Amritsar, Punjab-143005, India
*Corresponding authors: e-mail: tejwant.chem@gndu.ac.in

**Keywords**: Deep Eutectic Solvents, TGA, DSC, Supercapacitors

Thermally stable ionic soft materials or eutectogels based on a deep eutectic solvent (DES) of choline chloride and ethylene glycol (ChCl: EG) with a polyampholyte, gelatin (G), as a gelator have been prepared and characterized. The thermal stability of the prepared eutectogels has been investigated using the thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) techniques, respectively.

Depending on the gelatin content, the gels demonstrated robust mechanical features such as fast self-healing, great stretchability, strong *H*-bonding and thixotropic behavior. The produced gels have been examined for the presence of $\alpha$-helical structures using FTIR spectroscopy. The rheological characteristics of eutectogels, including their storage (G') and loss modulus (G''), have been analysed with respect to strain ($\gamma$), frequency ($\omega$), and temperature (T). The electrical properties of gels have been examined using cyclic voltammetry and electrochemical impedance spectroscopy, respectively. The eutectogel exhibits a 10-fold increase in electrical conductivity as compared to that observed in ethylene glycol-based gel, which decreases with an increase in the gelatin content. The gel scaffolds have been further investigated as stable electrolytes for supercapacitors. Owing to their greener and more facile preparation along with their multifunctional properties (self-healing, conducting, stretchable, multiadhesive, thixotropic, and antioxidant nature), these biosourced eutectogels could be utilised for different applications in daily life.[1,2]

**References**

[1] Z. Luo, W. Li, J. Yan, and J. Sun, *Advanced Functional Materials* 32 **(2022)** 2203988.
[2] G. Singh, G. Singh, K. Damarla, P. K. Sharma, A. Kumar, and T. S. Kang, *ACS Sustainable Chemistry and Engineering* 5 **(2017)** 6568-6577.

# Synthesis of highly luminescent $Eu^{3+}$and $Tb^{3+}$-doped hexagonal-phase $YPO_4$ nanoparticles with tunable emission at ambient Temperature

**LAISHRAM PETER SINGH, W. RAMESHWOR SINGH***

Department of Chemistry, Manipur University, Canchipur, Imphal, Manipur, India 795003
*Corresponding author: peterlaishramp@gmail.com

**Keywords**: Luminescent, Emissive, quantum-yield, h-phase

**Abstract:** Since luminous lanthanide nanoparticles are often made at high temperatures, these materials are expensive. Here, we're simply preparing one such substance at ambient temperature. $Tb^{3+}$ and $Eu^{3+}$ doped $YPO_4$ hexagonal phase nanoparticles allowed us to create green and red emissive nanoparticles. We were also able to adjust the emission color from green to yellow to red by adjusting the ratio of $Tb^{3+}$ to $Eu^{3+}$ energy transfer. By doping $Li^+$ ions into this system, we were able to triple the quantum yield while preserving the h-phase, despite the fact that this phase is said to be less emissive.

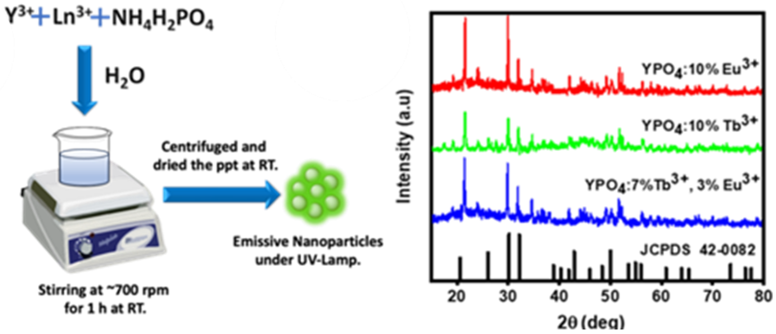


Fig. 1: Schematic representation for synthesis of Nanoparticle

**Reference**:

[1] A. Kar, S. Kundu and A. Patra, *ChemPhysChem*, 16 (**2015**) 505-521.
[2] A. Kar and A. Patra, *J. Nanosci. Nanotechnol.*, 18 (**2018**) 8047-8069.
[3] E. M. Surender, S. Comby, B. L. Cavanagh et al., *Chem*, 1 (**2016**) 438-455.

# Synthesis of Hydrogen Bonded Copper(II) Coordination Polymer: Photocatalytic Degradation of Rose Bengal Dye and Luminescent Sensing of Hg+2, Cr2O72−, and Nitrofurantoin

**ANAT RAM SIDAR[1], KAFEEL AHMAD SIDDIQUI[1]***

[1] Department of Chemistry, National Institute of Technology, Raipur, C.G. 492010, India
*Corresponding author: e-mail: *vshukla.phd2022.chy@nitrr.ac.in*

**Keywords**: Metal Organic Framework, Detection of Anion, Dye Degradation.

A new helical coordination polymer, $[Cu(Or)(H_2O)_3]_n$ has been synthesized at room temperature and examined using single-crystal X-ray diffraction (SC-XRD) and other analytical techniques. $[Cu(Or)(H_2O)_3]_n$ formed 1D helical type structure via coordination bonding as well as a 3D supramolecular network through hydrogen bonding interactions. $[Cu(Or)(H_2O)_3]_n$ manifested as a remarkable luminescent sensor for volatile organic compounds (VOCs), 3-Nitrophenol, $Cr_2O_7^{2-}$, $Hg^{2+}$, creatinine, nitrofurantoin and sucrose (200 mg/dl) in particular along with the remarkable photocatalytic degradation of Rose Bengal (RB) dye with 96.54% efficiency. Overall this study demonstrates that the synthesized Cu-orotate coordination polymer has good luminescent sensing and catalytic degradation activity, therefore could be employed for a range of applications such as sensing of biomolecules like sucrose and photocatalysis of toxic dyes.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Transforming biowaste *Calotropis procera pappus* into superhydrophobic material for organic solvent/oil-water separation

Priyadharshini[1], Mohammad Irfan[2], Chinthalapudi Naga Lakshmi[2], Narendra Singh[2]*

[1]Department of Chemical Engineering, Kalasalingam Academy of Research and Education, srivilliputhur, Tamil Nadu, 626126, India

[2]Department of Chemical Engineering, Indian Institute of Technology Tirupati, Tirupati, Andhra Pradesh, 517619, India

* Corresponding author. E-mail: narendra@iittp.ac.in

**Keywords:** Biowaste, Superhydrophobic/Superoleophilic, Surface modification, Oil-water separation

Oil-water separation is a global challenge, largely due to rising oil spill incidents during large-scale oil transportation and the substantial discharge of organic pollutants by industries. Developing materials to mitigate pollution in aqueous systems has become important. In this work, a sustainable solution for organic solvent and oil-water separation was achieved using *Calotropis procera pappus*, a readily available biowaste material. Surface modification with a blend of wax transformed the pappus fibers into a superhydrophobic material. The modified fibers exhibited a water contact angle (WCA) of 150.8°, indicating excellent water repellency. This *C. procera pappus*/ wax composite showed superhydrophobic and superoleophilic properties, with notable thermal stability (~50-200°C) and acidalkaline resistance (pH ~1-9). Characterization studies using FESEM revealed hierarchical structures in the pappus morphology contributing to super hydrophobicity, while ATR-IR and Raman spectroscopy depicted functional groups changes post-modification. Reduced BET surface area ($m^2/g$) for as modified *C. Procera pappus* sample, indicating successful surface functionalization. Thermal analysis via DSC and TGA demonstrated enhanced thermal stability. The developed material exhibited a high sorption capacity for organic solvents/oil (g/g) and showed reusability over 10 sorption cycles without significant performance loss. This material proved highly effective in separating organic solvents and oils from water, offering a sustainable solution for environmental remediation.

*18th International Congress on Thermal Analysis and Calorimetry, IITMadras, India,02-07 Sept. 2024*

# Characterization of conjugate between poly (N-vinyl caprolactam) and triazine-based covalent organic framework as potential biomaterial

**RASHMI PRABHA, PANNURU VENKATESU***

Department of Chemistry, University of Delhi, Delhi-110007, India.
*Corresponding author email: venkatesup@hotmail.com

**Keywords**: Thermoresponsive polymers, Poly (N-vinyl-caprolactam), Covalent organic framework, Biomaterials

Thermoresponsive polymers (TRPs) have been explored over decades for biomedical applications, and poly (N-vinylcaprolactam) (PVCL). TRP is extensively investigated due to low toxicity and a lower critical solution temperature (LCST) closer to physiological temperatures. Besides this, covalent organic frameworks (COFs) which belong to a class of porous polymers, their utilization in bio-based applications is of great interest due to their remarkable properties. Thus, integration of PVCL and COF as conjugate material can lead to advanced bio-based applications, but the need is to understand the influence of COF on the PVCL conformation. Herein, a triazine-based covalent organic framework (COF) i.e. CC-TAPT-COF has been synthesized and was completely characterized. Then the effect of CC-TAPT-COF on PVCL polymer conformation has been studied using various physicochemical techniques. Results from different studies showed a slight effect of CC-TAPT-COF on the PVCL conformation. On addition of CC-TAPT-COF concentrations slight decrease in LCST value for PVCL was observed. Studies revealed the presence of binding interaction between CC-TAPT-COF and PVCL, thus there was conjugate formation between them. The study will be beneficial for the development of COF- thermoresponsive polymer conjugates with a mixture of their unique feature as advanced biomaterials.

**References**

[1] R. Umapathi, K. Kumar, S. M. Ghoreishian, G. M. Rani, S. Y. Park, Y. S. Huh and P. Venkatesu, *ACS Omega*, 7 (**2022**) 39742–39749.
[2] P. Lavrador, M. R. Esteves, V. M. Gaspar and J. F. Mano, *Adv Funct Mater*, 31 (**2021**) 2005941.
[3] Y. Hiruta, *Polymer Journal*, 54 (**2022**) 1419–1430.
[4] N. A. Cortez-Lemus and A. Licea-Claverie, *Prog Polym Sci.*, 53 (**2016**) 1–51.

*18th International Congress on Thermal Analysis and Calorimetry, IITMadras, India,02-07 Sept. 2024*

# Investigation on the Performance of Nanofiber Coated Filter Media for Engine Applications

**SANGAMESH P SULIGAVI** [1*], **RAGHURAM CHETTY** [2], **ARUL PRAKASH KARAIYAN** [1]

[1] Department of Applied Mechanics and Biomedical Engineering, Indian Institute of Technology Madras, Chennai-600036, Tamil Nadu, India
[2] Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai-600036, Tamil Nadu, India
*Corresponding author: e-mail: am21d022@smail.iitm.ac.in

**Keywords**: Air filtration, Cellulose media, Nanofiber, Pressure drop, Quality factor

Air pollution has become an increasingly global issue due to industrial activity, traffic emissions, and urbanization. The subsequent haze catastrophes, widespread in developing countries like China and India, highlight the absolute need for efficient air filtration technology. Air filtration in vehicle internal combustion (IC) engines is crucial for maintaining optimal performance and prolonging engine life. It prevents contaminants from entering critical components, safeguards efficiency, and reduces wear and tear caused by pollutants.

Conventional cellulose fiber-based filters, though extensively used, demonstrate a reduced filter efficiency of aerosol particles in the range of $100 - 500\ nm$. Coating the cellulose media with nanofibers can improve the filtration efficiency at the expense of increasing pressure drop. Nylon-66 nanofibers possess a higher surface-to-volume ratio, good mechanical strength, and greater thermal stability. In the present study, an air filtration test rig with a suction type blower is employed, mimicking an IC engine intake. Nylon-66 nanofibers prepared by the electrospinning method coated over cellulose-based filter media were used for air filtration, with and without reduced graphene oxide (rGO). Experiments were conducted to evaluate the filtration efficiency, pressure drop, and quality factor (Q-factor) of the nano-coated filter media. This study addresses the ongoing research efforts to integrate nanofiber technology in air filtration systems. The air filtration efficiency is optimized with a corresponding reduction in pressure drop, thereby forming the crucial aspect in ensuring the system's performance.

18th International Congress on Thermal Analysis and Calorimetry, IITMadras, India,02-07 Sept. 2024

# Unravelling the role of gold nanoparticles modified by using ionic liquids having different anion on phase transition behavior of PNIPAM-b-PACMO

**SANJAY MOR[1], P. VENKATESU[1]***

[1]Department of Chemistry, University of Delhi, Delhi-110007, India
*Corresponding author: e-mail: venkatesup@hotmail.com

**Keywords**: Copolymerization, Stimuli-responsive polymers, Ionic liquid modified gold nanoparticles, Lower critical solution temperature

Utilizing stimuli-responsive polymers for surface modification of nanoparticle allows the adjustment of properties for individual system; however, limited research explores the impact of ionic liquid-modified gold nano particles (AuNPs) on the conformational phase transition of block copolymers. Herein, we synthesized poly(N-isopropylacrylamide)-b-poly(acryloylmorpholine) (PNIPAM-b-PACMO) copolymers by reversible addition fragmentation chain-transfer polymerization and investigated the effect of ionic-liquid modified AuNPs (IL-AuNPs) on the aggregation behavior of the copolymer. Copolymerization of PNIPAM with PACMO shifted the lower critical solution temperature (LCST) towards higher temperature in comparison to LCST value of PNIPAM. Addition of IL-AuNPs further raises the transition temperature in concentration dependent manner. A more significant alteration in the transition temperature was observed in the presence of IL-AuNPs with $Cl^-$ as an anionic part of the used ILs than that of $BF_4^-$ having same cationic part as 1-ethyl-3-methylimidazolium. The variation in transition temperature of the copolymer by different IL-AuNPs yields benefits in the temperature responsive properties which can helpful for various applications.

## References

[1] E. Cabane, X. Zhang, K. Langowska, C. G Palivan, W. Meier, *Biointerphases* 7 (**2012**) 1−27.
[2] K. Kumar, R. Yadav, and P. Venkatesu, J. *Phys. Chem. B,* 123 (**2019)** 6331−6344.
[3] K. Rao, K. Rao, C.S. Ha, *Gels*, 2 (**2016**) 2 6–25.

# "Mitigating Hydrogen Embrittlement in AHSS DP980: Efficacy of Nickel-Chromium Coatings in Preserving Mechanical Properties"

**ANJALI REGE[1], DR. MANISH VISHWAKARMA[12], TAUSEEF YAZDANI[2*]**

[1]Department of Mechanical Engineering, National Institute of Technology, Bhopal,
[2]Department of Mechanical Engineering, National institute of technology, Raipur, CG
MP
*Corresponding author: tauseefyazdani95@gmail.com

**Keywords**: Hydrogen embrittlement, coating techniques, UTM, SEM, zinc, Ni-Cr

This study aims to focus on hydrogen embrittlement in industrial steels especially on AHSS DP980 due to its wide range of application. It also focuses on chemical alterations to preserve mechanical properties. The study also considers coating techniques to maintain the material's integrity. Zinc and nickel- chromium coatings were in spotlight out of which nickel- chromium succeeds in preserving most of the properties. The samples were sampled according to the ASTM standards E8. UTM was conducted to investigate properties such as ultimate tensile stress, elongation, and fracture strength while SEM was conducted to investigate at micro levels. Highest ultimate strength is 1014.4 MPa and is recorded for bare, uncharged sample with elongation of 4 mm where as the result for Ni- Cr coated sample were ultimate strength of 960 MPa, 3.6 mm elongation which is approximately close to bare and uncharged sample. While on the other hand zinc coated and bare hydrogen charged samples were recorded to perform weakly due to interaction of hydrogen indicating high hydrogen content in steel which was converting it from ductile to brittle.

*18th International Congress on Thermal Analysis and Calorimetry, IITMadras, India,02-07 Sept. 2024*

# Batch Adsorptive Removal of Copper(II) from Aqueous Solution by Chitosan Oligosaccharide Nanocrystalline Cellulose-g-AM Hydrogel Composite

**GOVINDASAMY, SRINIVASAN LATHA***

Department of Chemistry, Vellore Institute of Technology, Vellore-632014, India
*Corresponding author: e-mail: srinivasan.latha@vit.ac.in

**Keywords**:

Designing green biocomposites for industrial wastewater treatment has gained more attention in the last few years. As a result of industrial activity, copper is one of the hazardous metals that is excessively found in water bodies and needs to be eliminated from the source. Multiple techniques have been developed to eliminate copper (II) metal ions from contaminated water (Lan et al., 2023). The exceptionally damaging potential of Cu (II) species makes them toxic metals. Chitosan oligosaccharide (COS), also known as low molecular weight chitosan, served as the foundation for the hydrogel biocomposite that was made in this work. Then, Ceric Ammonium Nitrate (CAN) was utilized as an initiator and crosslinker using Methylene Bis Acrylamide (MBA), and acrylamide as a monomer was used in the presence of nanocellulose (CL). The synthesized composite hydrogel, CS-CL – g – AM + MBA, was characterized by FT-IR, XRD, and SEM. The batch adsorption efficiencies in popular Cu (II) models were examined in order to assess the potential application of the composite (Pavithra et al., 2021). With an ideal pH of 6, a dosage of 5 gm, a time frame of 1 to 6 hours, and a metal ion concentration ranging from 25 mg/L to 1000 mg/L, the results demonstrate a promising elimination efficiency. The adsorption process extracted copper (II) ions from a copper-contaminated solution using a Freundlich isotherm mechanism and pseudo-second order kinetics. Consequently, the study's findings show that the developed composite is a very useful material for taking harmful contaminants out of water. Keywords: Chitosan Oligosaccharide, nanocellulose, hydrogel, Copper (II), Batch adsorption.

**References**

[1] Lan, X., Chen, J., Xie, Y., Hu, F., Chen, C., Li, D. & Deng, B. 28 (2023) 469.

# Development of Carbon Dioxide Capture unit for Diesel Engine

**MEHUL KALE, AJIT KUMAR PARWANI*, MAHUYA BANDHYOPADHYAY**

[1]Institute of Infrastructure Technology Research and Management, Ahmedabad 380026, India
*Ajit Kumar Parwani: e-mail: ajitkumar.parwani@iitram.ac.in

**Keywords**: Absorbent, $CO_2$ Capture, pH Values, Electrical Conductivity (EC) Value

Reducing the $CO_2$ emissions of the transportation sector stands out as one of the toughest challenges amidst the energy transition [1]. This research explores the efficiency of various absorbents, including Dimethylethanolamine (DMEA), Monoethanolamine (MEA), Calcium Hydroxide ($Ca(OH)_2$), and Potassium Hydroxide (KOH), in capturing $CO_2$ emissions from a single-cylinder diesel engine's exhaust running at constant speed of 1500 RPM. The absorbents demonstrated successful partial absorption of $CO_2$, leading to reduced emissions. MEA showed the highest $CO_2$ capture efficiency, followed by $Ca(OH)_2$, DMEA, and KOH the $CO_2$ emission on different loads using different absorbents as shown below in Fig.1. However, inconsistencies in emission reductions across different loads and time intervals suggest the influence of additional variables like temperature and pressure. Further studies are required to rectify measurement errors and optimize techniques for carbon capture technology development.

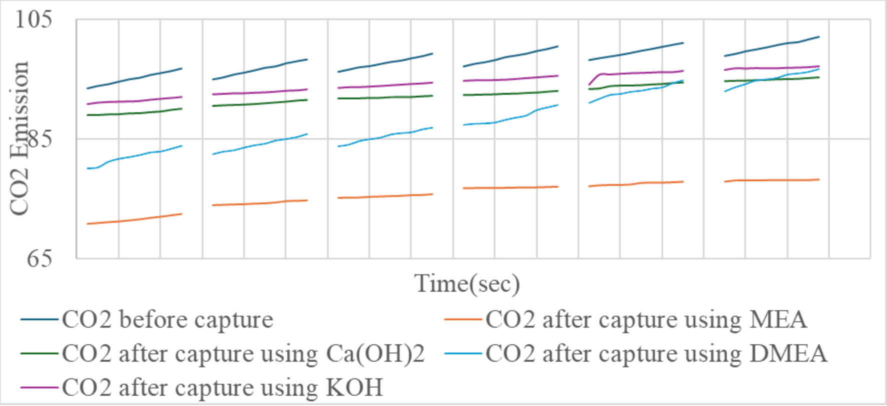


Figure 1:$CO_2$ emission before and after capture using different absorbents

## References

[1] Kumar, P., Rathod, V., & Parwani, A. K., *Environmental Progress & Sustainable Energy*, 40(5) (**2021**) e13651.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Examining $CO_2$ Capture in Hydrophobic Natural DES: Thermodynamic Properties and Environmental Screening

**Sinchan Hait, Upasana Mahanta[1]***
[1]Depertment of Chemical Engineering, BITS-Pilani K.K. Birla Goa Campus, Goa-403726, India
*Corresponding author: e-mail: upasanam@goa.bits-pilani.ac.in

## Abstract:

Anthropogenic carbon emission is a significant contributor to greenhouse gases. DES's tailor-making properties, low vapour pressure, and environmentally friendly properties make it an attractive medium for carbon capture. Considering energy consumption, hydrophobic DESs are the best alternative to their hydrophilic counterparts. This study uses a type-V hydrophobic natural DES (HNDES) as a solvent for carbon capture at 313.15K temperature and pressures up to 570 KPa. The eutectic composition of the DES mixture of menthol and camphor from COSMO-RS was 7:4 (molar ratio). Experimental Henry's constant, solubility, and $CO_2$ loading (α) were found to be 19.21MPa, 0.0232 (mole fraction), and 0.02074 (mole fraction). From COSMO-RS gas solubility, Henry's constant and density were calculated as 0.5084, 23.23MPa, and 0.913g/mL, respectively. Besides that, density, activity coefficient vapour pressure, Gibb's free energy of solvation, and environmental properties were computed using the COSMO-RS theory. The calculated Gibbs free energy (13.252KJ.mol$^{-1}$), enthalpy (-280.67 KJ.mol$^{-1}$), and entropy (-1KJ.mol$^{-1}$.K$^{-1}$) predict that $CO_2$ dissolution in DES is an exothermic and nonspontaneous process. Also, the toxicity of the individual components was screened through the Deep-PK web tool.

**Keywords**: Deep eutectic solvent, $CO_2$ capture, hydrophobic, COSMO-RS

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

---

# "Green Methods for Sustainable Zinc Metal Ion Extraction from Water Sources"

**SWATHI CHENNA[1]*, DHANALAKSHMI J[2]**

[1]Affiliation (institution only, see example)
[1,2] Solvent Development for Clean Technology Lab, Department of Chemical Engineering,
Sri Sivasubramaniya Nadar College of Engineering, Chennai – 603 110, India
*Corresponding author: e-mail: dhanalakshmij@ssn.edu.in

**Keywords**: Heavy metals, Zinc, Liquid-Liquid Extraction, Ionic liquids, Green Methods

Due to industrialization and globalization, millions of products have been produced, producing enormous amounts of wastes, and polluting the environment. As a result, organic and inorganic metals from industrial effluents have contaminated streams of water, making water scarcer and requiring the reusing of water after harmful materials have been adequately removed. One of the main contaminants in industrial wastewater is zinc, which can cause considerable physiological problems as well as possibly serious diseases in humans. Consequently, it is essential to remove zinc from wastewater efficiently. Although there are many ways to separate materials, liquid-liquid extraction has gained popularity due to its higher efficiency when compared to traditional techniques that have been documented in the literature. Initially performed using traditional organic solvents, the extraction process has evolved to incorporate ionic liquids in recent years due to their lower toxicity. This study investigates various separation methods for recovering zinc metals, focusing on analysing the essential parameters for optimizing its removal experimentally. The study highlights the importance of these initiatives are to improving human health and environmental sustainability.

**References**

[1] Anusha Basaiahgari, Ramesh L. Gardas, *Current Opinion in Green and Sustainable Chemistry* **(2020)** 100423.
[2] Xiaohua Li, Johannes J.M.M. van de Ven, Zheng Li, and Koen Binnemans, *Industrial. Engineering. Chemistry Research* **(2022)** 61, 17.
[3] Daniu Cai, Guangcai Zhang, Dongliang Hu,Jianyang Li, Minggong, *ACS Omega* **(2023)** 8,34.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Crack or Nuclei? What happens for pharmaceutical glasses annealed at low temperature?

**KOHSAKU KAWAKAMI**[1,2]

[1] Research Center for Macromolecules and Biomaterials, National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan, [2] Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Ibaraki 305-8577, Japan, e-mail: kawakami.kohsaku@nims.go.jp

**Keywords**: Pharmaceutical glass, nucleation, crystallization, crack

Glassy state is sometimes used for pharmaceutical development, as it has higher solubility compared to the crystalline state. Crystallization is not allowed to happen during both storage and dissolution for assuring its quality. Although deep cooling is known to enhance crystallization sometimes, its origin is still under debate.

We previously reported that nucleation proceeded under freezing temperature for celecoxib (CEL) glass [1], and it influenced dissolution [2] and stability [3] performances. However, effect of the crack formation on the crystallization behavior is also suspected [4]. We have repeated quench/annealing/reheating experiments for the CEL glass for more than four hundred times to find which factor, cracking and nucleation, plays dominant role for the crystallization. Fig. 1 shows probability of cracking and crystallization of CEL glass after annealing at various temperatures. Although high probability of the crystallization after deep cooling appeared to be associated with the cracking, crystallization could happen without cracking after the annealing at high temperature, indicating the influential role of nucleation. In the presentation, other evidences that suggested formation of nuclei at the freezing temperature range will be provided with similar observation for the loratadine glass.

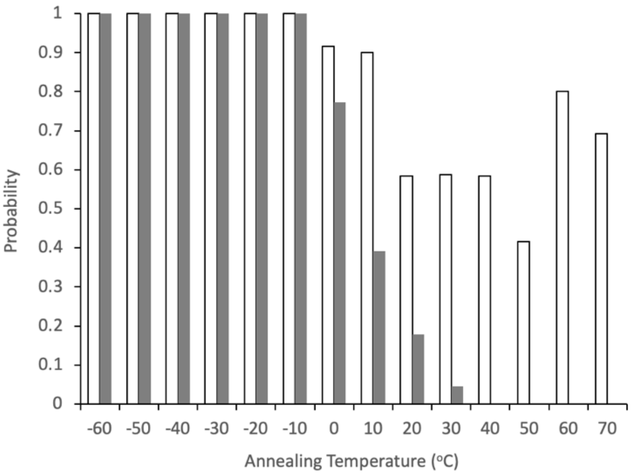


Fig. 1 : Probability of cracking (black) and crystallization (white) of celecoxib glass after annealing at various temperatures for one hour.

**References**

[1] K. Kawakami, *Thermochim. Acta*, 671 (**2019)** 43.
[2] J. Song, and K. Kawakami, *Mol. Pharmaceutics*, 20 (**2023**) 4050.
[3] X. Han, K. Dai, and K. Kawakami, *Mol. Pharmaceutics*, 21 (**2024**) 1794.
[4] S.D. Thakore et al., *Mol. Pharmaceutics*, 21 (**2024**) 76.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thymol encapsulated β-cyclodextrin for enhanced bio-efficacies

**DEBASHREE DAS[1]*, DHRITIMAN CHOWDHURY[2], ADITY BOSE[2], KAMALIKA SEN[1]**

[1]Department of Chemistry, University of Calcutta, Kolkata 700009, India
[2]Department of Chemistry, Presidency University, Kolkata 700073, India
*Corresponding author: e-mail: kamalchem.roy@gmail.com

**Keywords**: thymol, β-cyclodextrin, encapsulation, bio-efficacies, DNA binding

Thymol (Th) exhibits antimicrobial, antibacterial and antioxidant activity because of its phenolic structure. However, its clinical application in pharmaceutical industries is restricted due to its poor solubility and bioavailability. Cyclodextrin acts as a cost-effective drug delivery vehicle and guest molecules with suitable stereochemistry and polarity can be encapsulated inside its cavity. In the present study, different concentrations of thymol have been encapsulated in different concentrations of β-cyclodextrin at different time intervals according to Box Behnken design to obtain highest encapsulation efficiency (EE%) of thymol. The best encapsulation system (EE % 95.2) was found with 10 mM of β-cyclodextrin and 5.5 mM thymol at 6 h. Thymol encapsulated β-cyclodextrin was characterized by evaluating particle size, hydrodynamic radius and zeta potential using TEM and DLS. The enhanced bio-efficacies like improved solubility, sustained release, and higher affinity towards cancer cells like HeLa and MCF-7 than normal cells were observed due to encapsulation. The IC50 value of encapsulated thymol for MCF-7 cells was 200 µM which is lower than that of free thymol (300 µM), indicating improved anticancer activity of encapsulated thymol as well. The anticancer activity of thymol may be attributed to its DNA binding capability and subsequent degradation. Hence, DNA binding potentials of both free and encapsulated thymol have been further investigated using different spectroscopic, calorimetric, and theoretical studies.

**References**

[1] A. Kowalczyk, M. Przychodna, S. Sopata, A. Bodalska, and I. Fecka, *Molecules*, 25 (**2020)** 4125.
[2] S.Y. Raut, A.S.N. Manne, G. Kalthur, S. Jain, and S. Mutalik. *Curr Pharm Des*, 25 (**2019)** 444-454.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Effect of chitosan coating on liposomal encapsulation of cisplatin in a thin film hydration method

**TRIDIB BANERJEE[1], KAMALIKA SEN[1*]**

1Department of Chemistry, University of Calcutta, 92, APC Road, Kolkata 700009, India
*Corresponding author email ID: kamalchem.roy@gmail.com

**Keywords**: *in vitro* release, encapsulation, chitosan coating, Higuchi model

Liposomal systems are emerging as promising drug delivery systems as they consist of phospholipid membranes and display excellent drug loading capacity, drug protection, higher bioavailability, enhanced intracellular delivery, sustained release and greater therapeutic impact [1]. In the present study, cisplatin encapsulated liposomes were prepared via thin film hydration method by using soya-lecithin and cholesterol in $CHCl_3$/ MeOH mixture which has been coated with a bio-active polymer chitosan. The size and charge of these liposomal encapsulated systems have been characterized by dynamic light scattering (DLS) and zeta potential measurements. The morphology of these systems has been characterised by transmission electron microscopy (TEM). It has been observed that the size of these liposomal systems lie within the range 100-200 nm and *in vitro* release assay and encapsulation efficacy have been done by UV visible spectroscopic measurements. It has been observed that the release of cisplatin from liposomal encapsulated system was much slower compared to free cisplatin in ringer lactate medium and also the chitosan coating made the release of drug even much slower compared to the uncoated system. It has been observed that both the coated and uncoated liposomal systems followed non-fickian diffusion Higuchi model. Moreover, the chitosan coating also increased the encapsulation efficacy (99.74%) and stability of cisplatin encapsulated liposomal system compared to uncoated system (87%).

## References

[1] R. D. Hofheinz, S.U. Gnad-Vogt, U. Beyer, A. Hochhaus. Anti-cancer drugs, 16(7) (**2005**) 691-707.

# Thermodynamic Investigation of Molecular Interactions for Biosensing of Creatinine using β-cyclodextrin

**Swapnali S. Desai1[1], Mayur R. Parate1[1], Aatish S. Daryapurkar[1] and Dilip H. Dagade[2]***

*1Department of Electronics & Communication Engg. IIIT, Nagpur – 441 108*
*2Department of Chemistry, Shivaji University, Kolhapur – 416 004*
*Corresponding author: e-mail: dhd_chem@unishivaji.ac.in

**Keywords**: Osmotic and activity coefficient, hydration number, Virial Coefficient, KB integrals, Binding Constant, Biosensing.

Creatinine biosensing is a fast-emerging field due to creatinine's clinical significance as a key biomarker for thyroidal dysfunction as well as kidney and cardiovascular diseases. The thermodynamic studies of the molecular interactions are fundamental and essential to understand the behavior of the target analyte i.e. creatinine with other molecules. Seen in this light, the density measurements for binary aqueous solutions of creatinine and β-cyclodextrin (β-CD) were made at 310.15 K to probe the hydration and solute-solute interactions and the molecular level understanding of these were achieved through the osmotic pressure measurements using vapor pressure osmometer (VPO) for both the binary systems after analysis of water activity and activity coefficients data by means of application of statistical mechanical theories namely McMillan-Mayer (MM) theory and Kirkwood-Buff (KB) theory. Osmotic second ($NB2*$) and third ($N2B3*$) virial coefficients obtained were decomposed into repulsive and attractive parts contributing to solute-solute interactions. The limiting Kirkwood-Buff (KB) integrals $Gij0$ evaluated were also used to get the values of the $NB2*$ which shows an excellent agreement those obtained using MM theory.

Furthermore, the osmotic pressure measurements and analysis were made for ternary aqueous solutions of creatinine containing 0.01201 mol·kg−1 of β-CD and in the saline solution (0.1542 mol·kg−1) at 310.15 K. The data of transfer Gibbs free energy changes were subjected to scrutinize using MM theory to get the pair and triplet interaction parameters used further to determine the salting constant ($ks$) and equilibrium constant (log K = 3.05) for the β-CD-creatinine complex. The findings have been interpreted in terms of β-CD-Creatinine binding, hydrophobic interactions, and hydrophobic hydration in aqueous solution. The molecular level information on β-CD-creatinine aqueous system probed in this work and value of thermodynamic equilibrium constant based on activity measurements reported here for the β-CD-Creatinine complex will act as a fundamental information in the field of creatinine biosensing.

## References

[1] Kurhe, D. N.; Dagade, D. H.; Jadhav, J. P.; Govindwar, S. P.; Patil, K. J. *J. Solution Chem.* 40(6) (**2011)** 1596–1617.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Inhibiting the activity of mature Plasmepsin II from Plasmodium falciparum using fluoroquinolone-based antibiotics: Biophysical approach

**Sadaf Fatima Syed, Sinjan Choudhary***

UM-DAE Centre for Excellence in Basic Sciences, University of Mumbai, Vidhyanagri Campus, Kalina, Mumbai 400098, India.

*Corresponding author: e-mail: sinjan.choudhary@cbs.ac.in

**Keywords**: Plasmepsin, fluoroquinolone, enzyme kinetics, isothermal titration calorimetry (ITC), antimalarial therapy.

Plasmepsin II (PlmII) belongs to the aspartate proteases and is involved in hemoglobin (Hb) degradation in Plasmodium falciparum. Inhibition of mature plasmepsinII (mPlmII) activity is a promising strategy for antimalarial therapy, as it prevents Hb degradation, starving and ultimately killing the parasites. In this work, we have reported the inhibition of mPlmII activity by fluoroquinolones i.e. norfloxacin, ciprofloxacin, and sparfloxacin. The fluorescence spectroscopy and isothermal titration calorimetry (ITC) suggest all three fluoroquinolones bind to mPlmII with moderate affinity ($10^5$–$10^4$ $M^{-1}$) and the molecular docking result shows that only norfloxacin and ciprofloxacin bind at the active site of mPlmII via hydrogen binding and hydrophobic interactions. The thermodynamic parameters of binding of mPlmII with fluoroquinolones was studied using ITC. The enzyme kinetics studies demonstrate that norfloxacin and ciprofloxacin inhibit the activity of mPlmII with $IC_{50}$ values of 0.23µM and 0.32µM, respectively. Circular dichroism (CD) spectroscopy revealed minute alterations in mPlmII's structure upon increasing concentrations of the fluoroquinolones along with the change in thermal stability. Overall, the results here suggested that norfloxacin, and ciprofloxacin, can be repurposed as another source of antimalarial inhibitors targeting aspartic proteases. These physico-chemical and thermodynamic findings contribute to pave the way for potential therapeutic interventions targeted at malaria.

**References**

[1] T. M. Belete. Drug Des. Devel. Ther. 14 **(2020)** 3875-3889.
[2] T. D. M. Pham, Z. M. Ziora, M. A. T. Blaskovich, Med. Chem. Comm. 10 (10) **(2019)** 1719-1739.
[3]Tinku, S. Choudhary, J. Chem. Thermodyn. 177 **(2023)** 106951.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Application of DSC and TGA in exploring the temp induced changes in food and dairy products

**Sunil Meena[1*], B Keerthi Reddy[2], Anita Raj[1], Dinesh Chandra Rai[1,3], Raj Kumar Duary[1], and Priyae Brath Gautam[4]**

[1]Department of Dairy Science and Food Technology, Banaras Hindu University, Varanasi 221005, India
[2]Centre of Rural Development and Technology, IIT Delhi, New Delhi 110016, India
[3]B R A Bihar University, Muzaffarpur, 842001, India
[4]Department of Dairy Chemistry, SHAUTS, Prayagraj, 211007, India
*Corresponding author: Sunil Meena email: sunilmeena@bhu.ac.in

Food is considered as the most complex system due to its diverse composition and structural components. Thermal analysis techniques have been extensively used to investigate the impact of thermal processing on its constituents. In this study, techniques like DSC and TGA were explored, for evaluating the effect of different drying methods on *bathua* (*Chenpodium album*), an underutilized agricultural crop and effect of curcumin supplementation in Butteroil. Bathua being a highly perishable crop was preserved using sun, tray and freeze drying. The endo and exothermic peaks of the DSC analysis revealed the thermal degradation of the samples as indicated by the loss of primary phenolics and secondary metabolites in the powder samples. In addition, am inverse relationship was established between the glass transition temperature and water activity. Thermogravimetric profile of bathua powder samples reported that highest weight losses was occurred in freeze dried sample in 1st phase of heating (30-150°C), this loss may be attributed to the losses of water and volatile compounds during heating. The experiment conducted in temperature range of 30–700°C, and total weight losses of different samples was 67 – 68 % that may be due to water evaporation and thermal degradation of constituents (i.e., dehydroxylation, demethoxylation and decarboxylation reactions). In case of curcumin supplemented butteroil the thermograms appeared as a combination of exothermic and endothermic peaks in the control and curcumin-supplemented samples. During the melting process of butteroil, several endothermic peaks were detected that could be attributed to the distinct polymorphic crystalline forms of fat and the complicated structural composition of molecules in curcumin-supplemented butteroil. The thermal analysis for both the products facilitates in exploring the effect of thermal processing and supplementation of functional ingredients into the butteroil. The changes reported in the study have also been confirmed using NMR, FTIR analysis and surface morphology.

## Reference

[1] Reddy, B. K., Meena, S., Gautam, P. B., Meena, K. K., & Rai, *Microchemical Journal*, 201 (**2024**) 110537.
[2] Meena, S., Raj, A., Meena, J., Reddy, B. K., Rai, D. C., Duary, R. K., & Singh, G. P. *Food and Humanity*, (**2024**) 100316.

18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024

# Investigation of Calorific Values and Thermal Degradation Profiles of Various Plastic Wastes

**K.P.A. FAHMI**[1], **A. SHAIJA**[1]*, **N. BARANWAL**[1]

[1]Department of Mechanical Engineering, National Institute of Technology, Calicut, India
*Corresponding author: e-mail: shaija@nitc.ac.in

**Keywords**: thermo-gravimetric analysis, plastic waste, pollution, calorific value,

Plastic, a universal substance in our everyday existence, undergoes prolonged deterioration under climatic circumstances. There are seven types of plastics; Polyethylene terephthalate (PET), High density polyethylene (HDPE), Polyvinyl chloride (PVC), Low density polyethylene (LDPE), Polystyrene, and Polypropylene and 'others' which includes combination of resins. Out of the types mentioned, PET is not considered in this study as it is not available in pellet form in Kerala. Under Central Government, Plastic Waste Management Rule 2016 ammendment, PET bottles can not be recycled and used for food packaging applications. From the 'others' type, only multilayer plastic is considered in this study. Recycling encompasses four distinct categories; primary (recycling to same product), secondary (mixed colors or resins to different product), tertiary (waste to chemicals), and quaternary (waste to energy). Converting waste to energy is the ultimate method among aforementioned categories as it is utilizing waste as a fuel source. Study of the plastics' kinetics is the need of the hour to achieve optimal degradation results for a variety of processes. All types of plastics mentioned are collected in 0.5-1 cm pelletized form from various sources across Kerala. They varies in color, length and density depending on the recycling industry equipments and processes. Various parameters of plastics like calorific value (CV), degradation temperature, heating rate and byproducts of heating are found out using Bomb Calorimetry, Thermo Gravimetry mass Analyser (TGA) and Fourier Transform Infrared spectroscopy (FTIR) techniques. Average of three readings in different conditions are considered for calculation of CV. Compared to all the seven types of plastics, only PVC had some black residue in the bomb calorimeter while finding CV. This black residue is tested using FTIR. TGA was conducted on these seven types of plastics at various heating rates 10, 20, 30 and 40 °C/min which shows that kinetics of waste plastic degradation depends on the type of resin present in the polymer. It was found that mass profile ends below 600°C for polystyrene and LDPE, and it remains above 600°C for HDPE, PVC, polypropylene and multilayer plastic.

**References**

[1] A. O. Oyedun, C. Z. Tee, S. Hanson, *Fuel Processing Technology* 128 (2014), pp. 471–481.
[2] I. Dubdub and M. Al-Yaari , *Polymers* 12 (2020) 891.
[3] Z. Alhulaybi, I. Dubdub, *Polymers* 15 (2023) 3010.
[4] Y. Zhang, Z. Fu, W. Wang, G. Ji, M. Zhao, and A. Li, *ACS Sustainable Chemical Engineering.* 10 (2022) pp. 91−103.
[5] J.Yu, L. Sun, C. Ma, Y. Qiao, H. Yao, *Waste Management* 48 (2016) pp. 300–314.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Synthesis and characterization of novel cetyl pyridinium chloride – amino acid-based ionic liquids

**ROHIT KUMAR DEV[1], AJAYA BHATTARAI[*1], SUJIT KUMAR SHAH[1], RAMESH L. GARDAS[2], SHIV NARAYAN YADAV[1,3], MAHIMA KOIRALA[1], SRIJANA GHIMIRE[1], RIJAN GIRI[1], NISHA MAGAR[1]**

[1] Department of Chemistry, Mahendra Morang Adarsha Multiple Campus, Tribhuvan University, Biratnagar 56613, Nepal
[2] Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036, India
[3] Department of Chemistry, University of North Bengal, Darjeeling 734013, India
*****Corresponding author: bkajaya@yahoo.com

**Keywords:** cetyl pyridinium chloride, critical micelle concentration, ionic liquids, tuneable

The ionic liquids (ILs) are attracting much interest due to their numerous unique special qualities, such as being highly solvating, tuneable, non-flammable, and reusable extractants. This study reports an efficient synthesis of a novel set of room temperature ILs based on the active compound Cetyl Pyridinium Chloride (CPC) with amino acids [(AA= L-alanine, L-methionine, and L-valine)]. The synthesized ILs are characterized by their physicochemical and spectral analysis. These salts have been characterized by the following physicochemical properties: pH, conductivity, viscosity, density, boiling point, refractive index, and critical micelle concentration (CMC). Similarly, all synthesized ILs were described and compared with the existing samples using spectral analysis techniques like FT-IR, (1H &13C)NMR, and UV/Vis.

This present study provides an overview of the synthesis and characterization of ILs. The physicochemical and spectroscopic techniques characterize the ILs. Hence, this is a current area of research that is for the poise for the quick growth and development of the nation.

**Keywords:** cetyl pyridinium chloride, critical micelle concentration, ionic liquids, tuneable

## References:

[1] L. Peng, Z. Wang, H. Zhu, T. Zeng, W. Zhou, S. Yao, and H. Song. *Journal of molecular liquid*, 342(**2021**)116938
[2] M. Poterala, J. Plenkiewicz. *Tetrahedron: Asymmetry*, 22(**2011**)294-299
[3] L. Zuo, X. Ao. and Yu. Guo. *Journal of Chromatography A*, 1682(**2020**)461446

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Process optimization and modelling for the ozonolytic degradation of Atrazine

**A. KAVITHAKANI, K. CHITHRA***
Nanomaterials and Environmental Research Laboratory, Department of Chemical Engineering,
Alagappa College of Technology, Anna University, Chennai – 600025
* Corresponding author: chitrakumaran@yahoo.co.in

**Keywords**: Atrazine, ozonolysis, BBD, optimization & modelling

This study was carried out to treat Atrazine (Atz) a S-Triazine a class of pesticide. Atz transforms into micro-pollutant in aquatic systems because of its high solubility in water, low biodegradability and longer half-life making it to persist in water bodies for a longer time period leading to drastic pollution. Preliminary *insilico* docking studies was carried out using Autodock Vina to predict the binding affinity of Atz and ozone molecule for optimisation of process factors. The optimised conditions for the maximum degradation of Atz using the numerical mathematical optimisation (Box Behnken design (BBD) model) was explored in this work. Both the linear and the interactive effects of the process parameters were also studied using One Factor at a Time approach and Response Surface Methodology. On performing the BBD modelling the predicted maximum degradation of 75.66% occurred at pH-11, time of ozonation 11.397 minutes and the experimental % degradation was found to be 75.59% which proved the adequacy of the suggested model. FTIR analysis was done to confirm the breakage of complex ring structure of parent compound.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Design and Development of Sustainable Sports Shoes Using Recycled Materials in Compliance with Testing Standards

**LOGANATHAN T[1]*, AKSHAYA RAMAN M[2], DR. R. RAMAKRISHNAN[3]**

[1]Department of SFDP, FDDI, An Institute of National Importance, Hyderabad-500008, India
[2] Shoe & Product Design and Development Centre, CSIR - Central Leather Research Institute, Chennai–600 020, India
[3]Department of Sports Technology, Tamil Nadu Physical Education and Sports University, Chennai-600127, India
*Corresponding author: tloganathan@fddiindia.com

**Keywords**: Sustainable sports shoes, recycled materials, eco-friendly design, footwear industries.

This study delves into the design and creation of sustainable sports shoes using recycled materials that are aligned with the growing emphasis on eco-friendly practices in the global footwear industry. Our research prioritizes adherence to SATRA standards to ensure the quality and performance of sustainable sports shoes. Our findings underscore the effective utilization of recycled materials in sports shoe production offering not only environmental benefits but also meeting rigorous industry standards. This research provides valuable insights for industry professionals and researchers seeking to integrate sustainability into footwear manufacturing.

Globally, there is a growing trend in the usage of sports shoes.

Fig. 1: Visual Representation

**References**

[1] Van Rensburg, M. L., Nkomo, S. P. L., & Mkhize, N. M. *Waste Management & Research*, *38*(6) (**2020**) 599613.
[2] Roy Choudhury, A. K, *Roadmap to sustainable textiles and clothing: environmental and social aspects of textiles and clothing supply chain*, 1-39 (**2014**).
[3] SATRA Technology Centre. (2021). Footwear Testing Standards. Retrieved from www.satra.com

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Evaluation of Combustion Quality Index Using Graph Theory and Matrix Method

**NIKHIL DEV***

[1]J C Bose University of Science and Technology, YMCA, Faridabad-121006, India
*Corresponding author email id: nikhildevgarg@gmail.com

**Keywords**: Combustion, Index, Graph Theory, Matrix.

The Combustion Quality Index (CQI) is a qualitative metric to assess the effectiveness of combustion progressions in various combustion chambers. Factors such as fuel composition, combustion conditions, emissions etc assess combustion system performance. A high CQI designates efficient combustion with low levels of pollutants. Modifying fuel preparation, combustion chamber design, and operational parameters improve CQI. Therefore, qualitatively and quantitatively, continuous monitoring and control of these variables are essential. It is also beneficial for reducing environmental impact. One more index, the Carbon Aromaticity Index (CCAI), is similarly effective in assessing the ignition quality, pollution emission and combustion characteristics of residual fuel oils. A lower CCAI value also means better ignition quality, more efficient combustion and fewer emissions. The Third type of index acknowledged as the Calculated Ignition Index (CII) is used to evaluate the ignition quality of marine fuels, particularly residual fuels. The CII is typically used alongside other indices to provide a comprehensive evaluation of fuel quality.

In the present work graph theoretic approach (GTA) is used to evaluate CQI. The calculated value of the Combustion Quality Index (CQI) using GTMM (Graph Theory and Matrix Methods) is different from the one available literature and it can provide a structured and analytical way to assess the combustion process which are a part of the bigger system. This method involves representing the combustion system as a digraph and using matrices to analyse various aspects of the combustion process. In this approach, the components of the combustion system (e.g., fuel input, air input, combustion chamber, exhaust system, heat transfer system, cooling system etc) are represented as nodes in of a digraph. Afterward, the digraph is developed into a matrix using the matrix method. Combinatorial mathematics along with stanine is used to evaluate the matrix developed in the previous step. This methodology enhances flexibility and decreases complexity in the mathematical model. This approach also works to minimize complexity at different sub-system levels and during their operation. This type of mathematical tool is associated with many other benefits. If any new parameter or factor is to be incorporated into this model, then it can be done very conveniently. Because of this, computational cost is also not very much affected. As a result of the methodology followed as mention above, we obtain a numerical value, the combustion quality index for any combustion system which may be a complete system or a part of any big and complex system. The index values calculated with the mentioned methodology for the best and worst scenarios are calculated. It is found to vary from 2533470 to 1261870. For the calculation of index worth, a computer program developed in C+ is used with some modifications. Real-life situations will fall between these two extreme values. The index value allows us to make informed decisions on whether a component should be repaired or replaced or any other suitable change can be carried out.

## References

[1] N. Dev, Samsher, Kachhwaha, S S, R. Attri, *Ain Shams Engineering Journal*, 5(1) (**2014**) 193-203
[2] N. Dev, Samsher, Kachhwaha, S S, R Attri, *Ain Shams Engineering Journal*, 4 (**2013**) 273-284

*18th International Congress on Thermal Analysis and Calorimetry, IITMadras, India,02-07 Sept. 2024*

# A theoretical exploration into the associations among enablers and sustainable manufacturing technologies

**PRANAV GUPTE**[1]*

[1]Guru Ghasidas Vishwavidyalaya (A Central University), Bilaspur, Chhattisgarh
*Corresponding author e-mail: guptepranav01@gmail.com

**Keywords**: Sustainable manufacturing, technologies, enablers, correlation, natural resource based view, interconnectedness

The global manufacturing sector, while contributing significantly to economic growth, concurrently engenders detrimental impacts on environmental systems, precipitating crises related to global warming, climate change, and resource depletion among others. To address these challenges, manufacturing industries worldwide are increasingly adopting the concept of sustainable manufacturing (SM). SM entails the application of advanced and innovative methods, collectively known as sustainable manufacturing technologies (SMTs), to alleviate the adverse environmental effects of industrial operations. The adoption of SMTs is influenced by various factors acting as incentives towards their implementation, termed as enablers. There have been comparatively few studies that precisely explored the association among enablers and SMTs in manufacturing firms by broadly defining them, and no substantial management concepts have been utilized for supporting it. This research endeavors to fill this void by proposing a theoretical model grounded in the natural resource based view (NRBV) theory. The proposed model broadly categorizes SMTs and establishes correlations between them based on the interconnectedness principle of NRBV theory, which further divides the enablers into 'primary' and 'secondary' categories. By delineating this relationship, the study aims to offer valuable insights into the selection of specific SMTs in response to particular primary or secondary enablers within manufacturing firms and seeks to enhance the understanding of intricate dynamics governing the adoption of SMTs in manufacturing sector.

**References**

[1] M. Aboelmaged, *Journal of Cleaner Production*, 175 (**2018**) 207-221.
[2] O. Fatoki, *Academy of Entrepreneurship Journal*, 25 (**2019**) 1-12.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

---

# Investigating the effect of temperature on carbon dioxide adsorption capacity of amine-modified clay

**PRATIBHA SHARMA[1], RAJU KUMAR GUPTA[1]*, HIMANSHU SHARMA[1]***

[1]Department of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur-208016, India
*Corresponding author: e-mail: guptark@iitk.ac.in, sharmah@iitk.ac.in

**Keywords**: carbon dioxide capture, temperature effect, clay adsorbents, amine modification

The substantial release of $CO_2$ from the combustion of fossil fuels profoundly affects Earth's climate. $CO_2$ capture, utilization, and sequestration techniques aim to mitigate this by capturing $CO_2$ from its source which can then be utilized to produce value-added products or injected in the subsurface reservoirs for long-term storage. Currently, amine-based solvents are used to capture $CO_2$ but this process is energy-intensive, expensive and environmentally unfriendly.

In our research, we investigated the potential of utilizing readily available, environmentally friendly and low-cost materials such as clays to develop porous solid adsorbents for $CO_2$ capture. The synthesis process involves the thermal and base treatment of clay through a hydrothermal process to increase its porosity and surface area. This pre-treated clay was then utilized as a new type of support for amine impregnation to further enhance $CO_2$ adsorption. The $CO_2$ adsorption capacity of these adsorbents was investigated using thermogravimetric analysis. It was found to be 0.136 mmol/g for pre-treated clay which increased to 0.83 mmol/g for amine-impregnated clay at 25°C with an optimal amine loading of 50 wt%. The effect of temperature on $CO_2$ adsorption capacity of these adsorbents was also investigated by varying the temperature from 25°C to 65°C to identify the optimum temperature for $CO_2$ adsorption. The synthesized adsorbents were characterized by scanning electron microscopy, elemental analysis, $N_2$ physisorption, and Fourier transform infrared spectroscopy. The effect of various factors such as pore size, and amine loading on $CO_2$ adsorption capacity was also studied. The combination of good $CO_2$ adsorption capacity and cost-effectiveness of the amine-modified clay-based adsorbents suggest that the clay minerals have the potential to be employed as economically efficient adsorbents to capture $CO_2$.

# Development of Leather Waste Composite Sheets as Sustainable Material for Upholstery Applications
## Abstract for ICTAC 2024

**RAJESH CHENGAMCHETTY MURALI[1], AKSHAYA RAMAN M[1], DR. MATHIVANAN S[1*], SURESHKUMAR D[1]**
Shoe and Product Design Development Centre, CSIR – Central Leather Research Institute, Chennai600020, India
*Corresponding author: mathivanan@clri.res.in

**Keywords**: Leather waste composite, Sustainable materials, upholstery, compression moulding

The paper focuses on developing leather waste composites by pulverizing leather dust and manufacturing scraps, then mixing them with additives like polyurethane (PU) and silicone-based polymers to create sustainable upholstery materials. These composites, particularly the 80/20 PU/leather blend, exhibit superior mechanical properties, including a tensile strength of 3.0595 N/mm², significantly outperforming conventional materials. The composites demonstrate reduced water absorption, stable electrical properties, and improved fire resistance, with a Limited Oxygen Index (LOI) of 24 and a delayed ignition time of 8 seconds. This innovative approach not only addresses practical concerns for aircraft interiors but also aligns with environmental goals, promoting a circular economy and carbon reduction in the aviation industry.

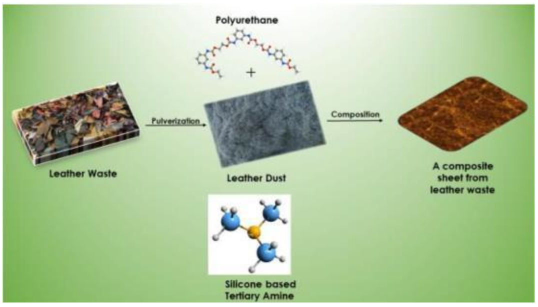


Fig. 1 : Graphical Abstract

**References**

[1] K. Bartoszuk & A. Wronka, *Annals of WULS, Forestry and Wood Technology*, (**2023**) 124-134.

[2] K. Bartoszuk, G. Kowaluk, *Materials*, 16 (**2023**) 5340.

[3] D. Santos, Renivaldo & Agostini, Deuber & Cabrera, Flavio & Budemberg, Eduardo & Job, Aldo. *Polymer Composites*, 36 (**2015**) 2275-2281.

[4] U. Akı, S., Candan, C., Nergis, B., & Sebla Önder, N. Understanding Denim Recycling: A Quantitative Study with Lifecycle Assessment Methodology. IntechOpen.2020

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Extractive Removal of Dyes from Industrial Effluent: A Circular Approach Employing Pseudoprotic Ionic Liquids

**SACHIND PRABHA PADINHATTATH, JEGAN GOVINDARAJ, RAMESH L GARDAS***

Department of Chemistry, Indian Institute of Technology Madras, Chennai 600036, India
*Corresponding author: e-mail: gardas@iitm.ac.in

**Keywords**: Ionic liquids, Dyes, Industrial effluent, Reuse

The uncontrolled discharge of dye effluents from various industries into aquatic environments poses a significant challenge. Conventional wastewater treatment methods often fall short in treating these effluents due to their lack of specificity and the potential formation of secondary pollutants[1]. To address this issue, a novel method was developed to test the efficacy of pseudoprotic ionic liquid (PPIL) based liquid-liquid extraction (LLE)[2] for the effective removal of different categories of dyes from both simulated and real industrial wastewater samples[3]. Through a thorough screening, it was determined that a PPIL formed by combining an equimolar mixture of tricotylamine (TOA) and octanoic acid (OA) is capable of extracting anionic dyes from simulated wastewater samples. All extraction experiments were conducted under controlled conditions at pH 7±0.1 and 303.15±1K, with systematic optimization of key parameters affecting the extraction process. Furthermore, adjustments to the organic acid to base mole ratio led to changes in the physical properties of the PPIL[4]. At a molar ratio of TOA:OA (1:9), the PPIL was found to be effective in extracting cationic dyes. In both cases, the back-extraction of dyes from the PPIL-rich phase was carried out using appropriate stripping agents, which enabled the solvent to be reused for multiple extraction cycles. Following the favourable results obtained from simulated samples, the developed methodology was applied to real industrial effluent collected from the Angeripalayam Common Effluent Treatment Plant (ACETP) in Tirupur, Tamil Nadu, India. The application demonstrated the PPIL's capability to efficiently remove vinyl sulphone dyes from real industrial samples, affirming its potential for practical use in industrial wastewater treatment.

**References**

[1] G. Bal and A. Thakur, Mater.Today Proc., 50 (**2022)** 1575-1579.
[2] C. H. C. Janssen, Ind. Eng. Chem. Res., 60 (**2021**) 1808-1816.
[3] S. P. Padinhattath, J. Govindaraj, R. L. Gardas, J. Water Process Eng., 58 (**2024**) 104921.
[4] M. N. Kobrak and K. G. Yager, Phys. Chem. Chem. Phys., 20 (**2018**) 18639-18646.

# Solid Phase Recovery of Valuable Metals from Electronic Waste

**SRINIVASARAO KANCHARLA[1]*, KARTHIGA P[1], RAJENDRAN M[1],**
**SAJITH BABU M K[1], MADHUMITHA M[1]**

[1]Department of Chemistry, SRM Institute of Technology, Kattankulathur-603202, Tamil Nadu, India
*Corresponding author: e-mail: srinivak5@srmist.edu.in; sreeksrinivasarao@gmail.com

**Keywords**: Metal recovery, e-waste, leaching, sorption, precipitation

Electronic waste (e-waste) is the fastest-growing type of solid waste globally due to the increased usage and shortened lifespans of electronic devices. In 2021, the generation of e-waste exceeded 54.8 million tonnes (MT) worldwide, with projections indicating it could reach 74.7 MT by 2030 [1]. E-waste contains several valuable metals, including copper (Cu), gold (Au), iron (Fe), tin (Sn), and nickel (Ni). Among these, Cu and Au are particularly noteworthy. Cu makes up approximately 20% of the composition of electronic equipment due to its exceptional thermal and electrical conductivity, while Au is highly prized for its increasing demand and value.

Hydrometallurgy is the most followed method for metal recovery from e-waste, offering advantages over pyrometallurgy. Solid-phase recovery is a beneficial approach within hydrometallurgy, and it can be carried out using three methods: (i) Direct leaching of metals from e-waste using suitable functionalized insoluble solid materials [2]. (ii) Selective extraction of metals from leachates using functionalized materials. (iii) Precipitation of metals from leached liquors using suitable small molecules. This presentation will discuss the recovery of metals from e-waste using these three methods. The focus will be on the utilization of biopolymers and carbon materials for recovering Cu(II) from printed circuit board waste, as well as the detailed recovery of Au(III) by precipitation from CPU pin leachates.

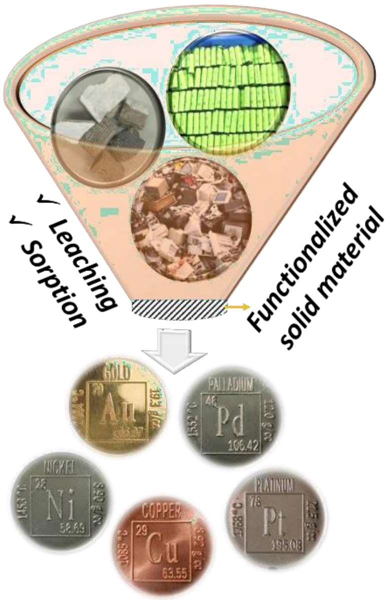


Fig. 1. Schematic overview of the recovery of valuable metals from waste.

**References**

[1] G. M. Massa, V.-M. Archodoulaki, *Environments* 10 (**2023**) 44.

[2] M. Manickasundaram, K. Lakshmanan, K. Vediappan, S. Kancharla* *Chem. Eng. J.* 484 (2024), 149605.

# Fe-doped Zinc-MOF Composites and its Test-Strip Employed for Colorimetric Detection of Glucose in Model and Real Urine Samples

**VIBHAV SHUKLA[1], KAFEEL AHMAD SIDDIQUI[1]***

[1] Department of Chemistry, National Institute of Technology, Raipur, C.G. 492010, India
*Corresponding author: e-mail: *vshukla.phd2022.chy@nitrr.ac.in*

**Keywords**: Metal Organic Framework, MOF-Composite, Detection of Glucose, Urine Sensing.

We present an innovative luminescent probe based on a novel Metal-Organic Framework (MOF), $\{[Zn3(Cei)2(COO)2(Bimb)3]\cdot C2H2\}n$ (Zinc-MOF), and its iron-doped composite (Fe@Zinc-MOF), meticulously designed for glucose detection. The structural integrity and performance of these composites were validated through comprehensive analytical techniques. The probe demonstrated exceptional linear correlation coefficients ($R^2 = 0.97118$) for glucose concentrations of 110 and 150 mg/dl. Impressively, the Stern-Volmer quenching constants (Ksv) at low glucose concentrations were determined to be $3.2 \times 10^4\ M^{-1}$ and $3.8 \times 10^4\ M^{-1}$ in real urine samples. The probe achieved remarkable detection limits of 1.17 ppm and 0.846 ppm for 110 and 150 mg/dl glucose, respectively, in real urine samples. To further enhance practicality, a highly sensitive detection strip was fabricated using filter paper impregnated with the Fe@Zinc-MOF composite. This strip exhibited significant fluorescence changes corresponding to varying glucose concentrations, underscoring its potential for ultra-sensitive glucose monitoring. Our findings pave the way for advanced, real-time glucose detection in clinical diagnostics, offering a promising tool for efficient health monitoring.

T8- OP 12

# Numerical analysis of $LiFePO_4$ battery wall temperature with air cooling using copper metal foam

**ARJUN P S[1]*, D ARUMUGA PERUMAL[2]**

Department of Mechanical Engineering, National Institute of Technology Karnataka, Surathkal-575025, Karnataka, INDIA
*Corresponding author: e-mail: perumal@nitk.edu.in, Ph: +9159860535

**Keywords**: Lithium-Ion battery; Mixed convection; Darcy extended Forchheimer model (DEF); Local thermal non-equilibrium (LTNE)

This study focuses on the computational analysis of heat dissipation from open-cell copper metal foam that cools $LiFePO_4$ battery packs. Metal foams with air as a working fluid are gaining increased attention for managing the heat dissipation from lithium-ion batteries [1, 2]. In this study, various samples of copper metal foams are placed between vertically arranged $LiFePO_4$ battery modules [Fig. 1]. The properties of the $LiFePO_4$ battery cells are derived from existing data. The work examines mixed convection heat transfer through vertically positioned metal foams to analyze fluid flow and heat dissipation characteristics for different mass flow rates. The Darcy-extended Forchheimer (DEF) model is employed to study fluid flow through metallic foams, and the local thermal non-equilibrium (LTNE) model is used to understand heat transfer characteristics. The study also investigates the variations in heat transfer for lithium-ion battery modules at different pore densities. The results indicate that copper foam with appropriate porosity and pore density can effectively cool the $LiFePO_4$ battery pack.

Fig. 1: Illustration of copper foam on battery module.

**References**
[1] P.S. Arjun and D.A. Perumal, *Recent Patents on Mechanical Engineering*, 17 (**2024**) 196.

*18th International Congress on Thermal Analysis and Calorimetry, IITMadras, India,02-07 Sept. 2024*

# Volumetric Studies of Theophylline-PEGylated Deep Eutectic Solvent in Aqueous Solution

**VICKRAMJEET SINGH*[1] ARPITA PADHAN[1], ANSHUMAN PATTANVALLA[1], SHIKHA INDORIA[2]***
[1]Department of Chemistry, Dr. B. R. Ambedkar National Institute of Technology, Jalandhar 144027, Punjab, India.
[2]Department of Chemistry, School of Chemical Engineering and Physical Sciences, Lovely Professional University, Jalandhar, 144411.
*Corresponding author: e-mail: singhvj@nitj.ac.in; shikhao87@yahoo.com

**Keywords**: Deep eutectic solvent, theophylline, thermodynamics, interactions

Deep eutectic solvents (DESs) have gathered significant attention as eco-friendly alternatives to conventional solvents. Understanding the solution chemistry of DES is crucial for green chemistry processes to pharmaceutical formulations. This study presents a comprehensive volumetric investigation to elucidate the molecular interactions and thermodynamic properties of theophylline in aqueous DES environments. A DES composed of PEG-400 and citric acid/ascorbic acid was tailored to study theophylline-DES interactions. Measurements of density and speed of sound were conducted within the range of (293.15−318.15) K and 0.1 MPa, while UV-visible studies were performed at 298.15 K. Analysis of apparent molar volumes, infinite dilution partial molar volumes, and volumetric transfer parameters provided insights into the solute−solute, solute−solvent, and solute−cosolute interactions between theophylline and DES in aqueous environments. The findings indicate a complex interplay of interactions among DES components and theophylline, with notable observations on the dimerization of theophylline leading to a reduction in absorbance with increasing co solute concentration. This study sheds light on DES-mediated drug solubilization's molecular dynamics, offering valuable implications for pharmaceutical applications.

# Thermophysical Properties of Arabian sea for Feasibility of Desalination Plants in Estuarine Systems.

NISHABEN DESAI DHOLAKIYA[1]*, ANIRBAN ROY[1], RANJAN DEY[2]

[1]Department of Chemical Engineering, BITS Pilani Goa, Goa 403726, India
[2] Department of Chemistry, BITS Pilani Goa, Goa 403726, India
*Corresponding author: p20210046@goa.bits-pilani.ac.in

**Keywords**: Estuarine systems, Thermodynamic, Thermoacoustic, Arabian Sea.

In the Indian context several metropolitan and growing cities are experiencing moderate to severe water shortages [1]. In order to provide water security to the entire nation, desalination plants need be installed and commissioned [2] along the coastal cities. The coastal tract in the state of Goa lies between 14°48' N and 15°48'N and between 75°40'E and 74°20'E, lying adjacent to the Konkan coast of Maharashtra [3]. It is important to note that very little study has been done on the feasibility of desalination plants in estuarine systems. Understanding the variation in salinity becomes extremely crucial in the context of a techno-economic analysis [4].

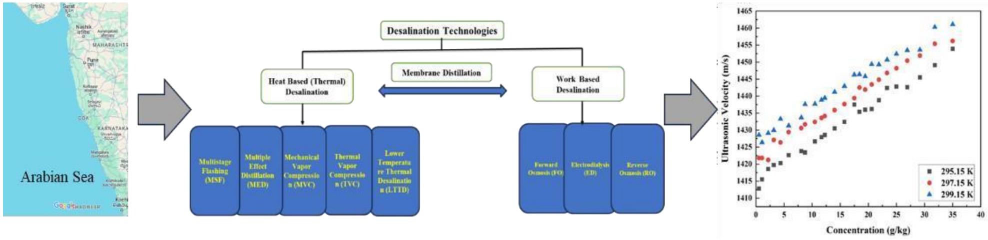


Figure 1 Schematic model of desalination technologies aided by thermophysical properties.

To bridge this gap, this investigation probes the ultrasonic velocity, density and thermoacoustical parameters of raw sea water of Arabian sea, Goa (India) at various temperatures. Thermophysical properties have been evaluated using the experimental values. The findings will pave the thermodynamic feasiblity of setting up of desalination plants in the coastal regions of India

## References

[1] S.K. Jain, Providing water security in India by conserving and utilizing flood flows, Water Security 14 (2021). https://doi.org/10.1016/j.wasec.2021.100105.

[2] R. Rath, A. K. Ghosh, & A. Roy, (2022). Sustainable Desalination: Future Scope in Indian Subcontinent. Sustainable Water Treatment: Advances and Technological Interventions, 567590.

[2] S. N. Karlekar, S. C. Thakurdesai, and A. Kar. "Geomorphological field guide book on Konkan and Goa Coasts." In Ninth International Conference on Geomorphology of the International Association of Geomorphologists. New Delhi: Indian Institute of Geomorphologists, 36p. 2017.

[4] L. M. Rehman, R. Dey, Z. Lai, A. K. Ghosh, & A. Roy, *Industrial & Engineering Chemistry Research*, 59(36) (**2020**) 16029-16042.

# Intermolecular interaction studies of DMSO/NMP+Water Systems at varying temperatures

**PRASEEDA P NAIR**[1], **ADITI PRABHUNE**[1], **RANJAN DEY**[1*]

[1] Department of Chemistry, BITS Pilani KK Birla Goa Campus, Goa-403726, India

*Corresponding author: e-mail: ranjandey@goa.bits-pilani.ac.in

Keywords: Thermophysical, Binary, Excess properties, Intermolecular interactions

Thermophysical properties of binary solutions provide critical insights into the intermolecular interactions prevalent in binary and higher order mixtures. In the present investigation, thermodynamic and transport properties viz density, ultrasonic velocity, coefficient of thermal expansion, adiabatic compressibility and their excess counterparts together with deviations in ultrasonic velocity and viscosity have been determined over a temperature range of 293.15 K to 318.15 K for binary mixtures of Dimethyl Sulfoxide (DMSO) with water and N-Methyl Pyrrolidone (NMP) with water. The findings have been used to understand the nature and extent of the intermolecular interactions prevalent in the systems under investigation. The comparative study of these binary mixtures sheds light on these underlying molecular interactions and their role in influencing thermodynamic behaviour.

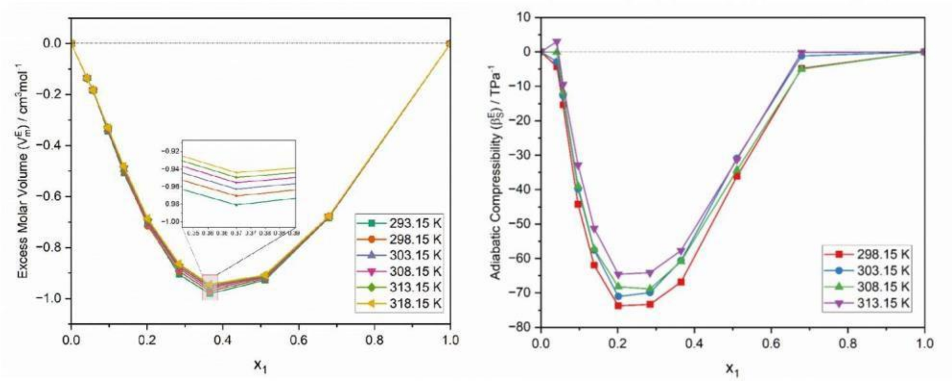


Fig. 1 : (a) Excess Molar Volume of DMSO + Water at various T
(b) Excess Adiabatic compressibility of DMSO + Water at various T

References

[1] A. Basarkar, R.Dey, *Journal of Molecular Liquids*, (**2022**) 367:120457.
[2] A. Prabhune, A. Natekar, R.Dey, *Frontiers in Chemistry*, (**2022**) 10:868836.
[3] Saini A, Prabhune A, Mishra AP, Dey R, (**2021**) 323:114593.

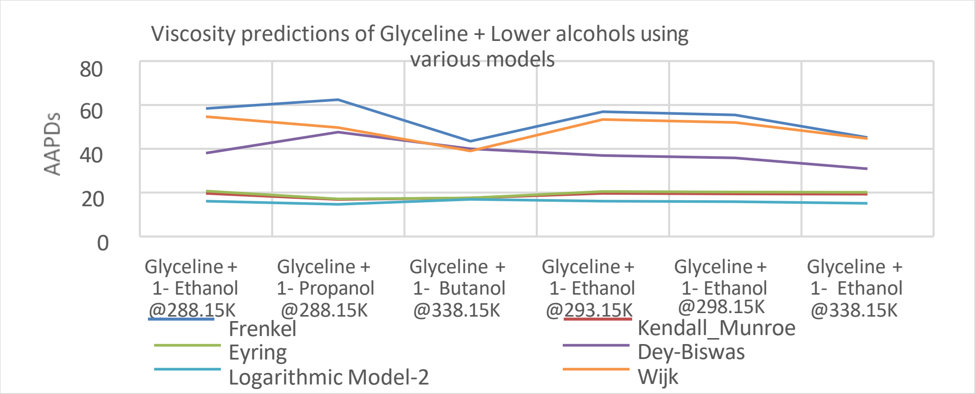
*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermophysical properties of DES, Glyceline with $C_2$-$C_4$ alcohols at varying temperatures

SURAZ KUMAR*, RANJAN DEY

Department of Chemistry, (BITS) - Pilani, K. K. Birla Goa Campus, Zuarinagar, Goa, India-403726.
e-mail ID: f20211602@goa.bits-pilani.ac.in ; ranjandey@goa.bits-pilani.ac.in

Deep eutectic solvents (DES) are mixtures of two or more pure components, typically containing at least one hydrogen bond donor (HBD) and one hydrogen bond acceptor (HBA) which interact amongst themselves to form a eutectic mixture. The key feature of DES is the significant drop in the freezing point of the mixture when compared to its constituent pure components due to the formation of an extended complex hydrogen bonding network. The study of these solvents is very crucial due to their varied applications in different fields like chemical, pharmaceutical, and petrochemical industries among some more industries too. Some specific uses of DES include its usage in drug delivery processes and electroplating.

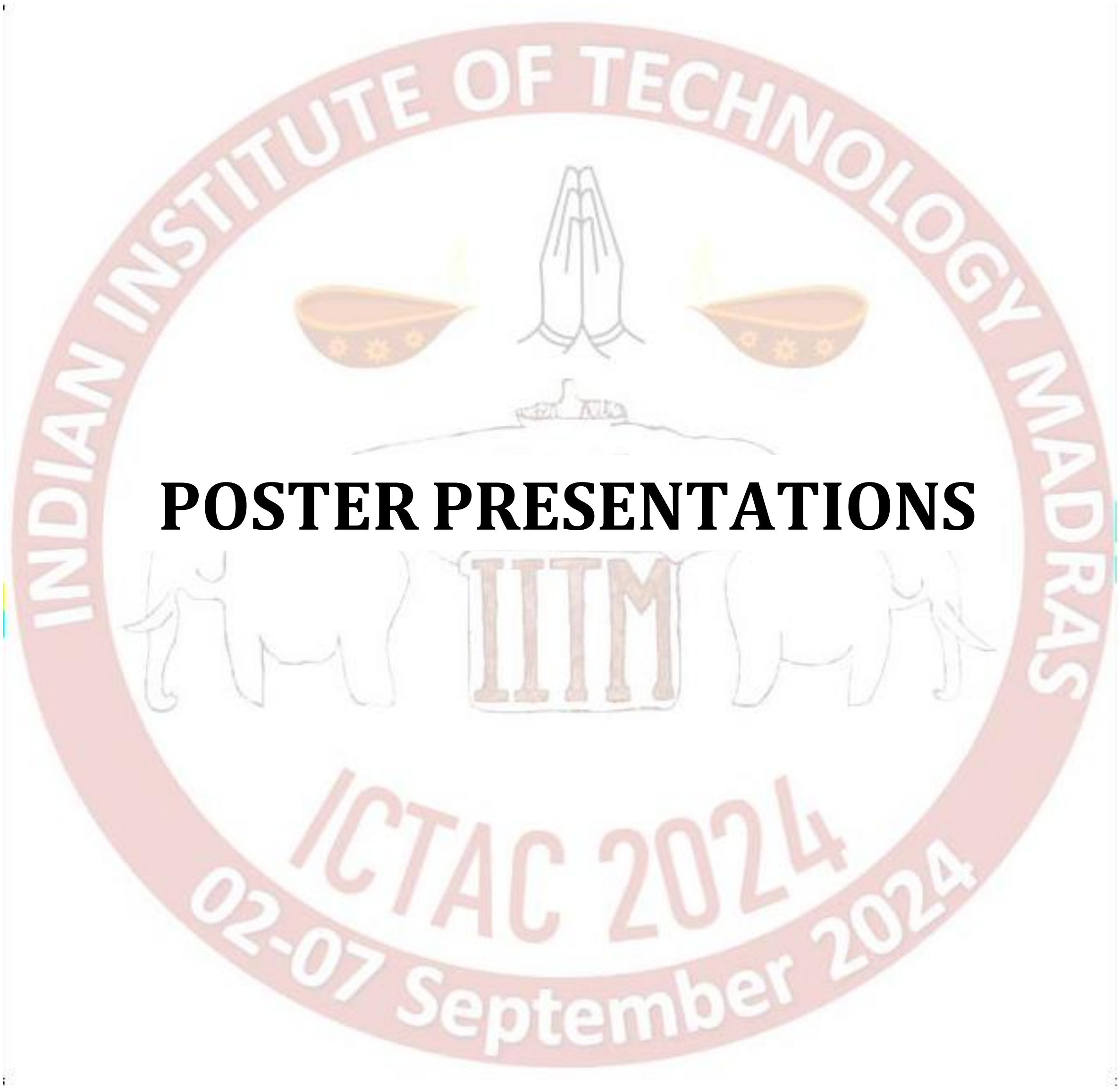


In the present investigation, an attempt has been made to evaluate the coefficient of thermal expansion (α), excess thermal expansion coefficient ($\alpha^E$), the interaction parameter of the Glyceline and alcohols at various temperatures. Comparative studies of ultrasonic velocity and viscosities by different models have been carried out. The experimental values have been taken from literature[1].

References:

1. Guadalupe Perez-Duran, Gustavo A. Iglesias-Silva, Jose Julian Cano-Gomez, Mariana RamosEstrada, J. Chem. Thermodynamics 193 (2024) 107264.
2. Akanksha Saini, Shashwat Verma, Aditya Harshavardhan and Ranjan Dey, RSC Adv., 2016, 6, 113657. 3. Ranjan Dey, Aditya Harshavardhan, Shashwat Verma, Journal of Molecular Liquids 211 (2015) 686-694.
4. Ranjan Dey, Piyashi Biswas, Journal of Molecular Liquids 265 (2018) 356-360.
5. Aditi Prabhune, Ranjan Dey, Journal of Molecular Liquids 379 (2023) 121676.

# POSTER PRESENTATIONS



*18th International Congress on Thermal Analysis and Calorimetry, IITMadras, India,02-07 Sept. 2024*

# Dielectric Response of Solvents Using Molecular Simulations

**SRIKANTH DIVI[1]*, ANOOP KISHORE VATTI[1], TAMAL BANERJEE[2]**

[1]Department of Chemical Engineering, Manipal Institute of Technology (MIT), Manipal Academy of Higher Education (MAHE), Manipal, 576104, Karnataka, India
[2]Department of Chemical Engineering, Indian Institute of Technology Guwahati, Guwahati, 781039, Assam, India.
*Corresponding author: e-mail: tamalb@iitg.ac.in

**Keywords**: Organic solvents, dipole moment, static dielectric constant, DFT, classical MD

Accurate prediction of organic solvent properties is a critical challenge using molecular simulations. These solvents are crucial components in batteries, and their properties significantly influence performance. Therefore, reliable methods and levels of theory are needed to predict refractive index, static dielectric constant, and electronic polarizability. As battery technology advances, optimizing electrolyte properties, such as dielectric constant and viscosity, becomes crucial for enhancing energy density, power output, and safety. Quantum mechanical calculations accurately determine the charge distribution within individual electrolyte molecules composed of organic electrolytes. Molecular dynamics (MD) simulations are performed to accurately predict N-Methyl-2-pyrrolidone, dimethoxyethane, and ethylene carbonate. These results confirm that the prediction of macroscopic effects from molecular dynamics simulations can effectively mimic the dielectric constants, refractive index, electronic polarizability and dielectric constant of organic solvents.

*18th International Congress on Thermal Analysis and Calorimetry, IITMadras, India,02-07 Sept. 2024*

# Thermal Conductivity and Stability of Cyrene Nanofluid using Molecular Dynamics Simulations

**ANOOP KISHORE VATTI[1], TAMAL BANERJEE[2]***

[1]Department of Chemical Engineering, Manipal Institute of Technology (MIT), Manipal Academy of Higher Education (MAHE), Manipal, 576104, Karnataka, India
[2]Department of Chemical Engineering, Indian Institute of Technology Guwahati, Guwahati, 781039, Assam, India.
*Corresponding author: e-mail: tamalb@iitg.ac.in

**Keywords**: Cyrene, Carbon Nanotubes, Nanofluids, Reverse NEMD, Thermal Conductivity

## Abstract:

Cyrene, which is frequently known as Dihydrolevoglucosenone, is a biodegradable solvent that is employed in a variety of applications such as alternative solvent in chemical reactions, and in heat transfer applications. To improve the thermal characteristics of the biodegradable solvent by utilizing nanoparticles, it is essential to accurately predict the thermal conductivity and viscosity of the solvent Using molecular dynamics simulations, we simulated a nanofluid by utilizing both pristine carbon nanotubes and surface-functionalized carbon nanotubes in cyrene, such as carboxyl (-COOH) and amine ($-CO-NH(CH_2)2NH_2$) groups using reverse non-equilibrium molecular dynamics simulations. Finally, we have investigated various structural, dynamical and thermal properties of the cyrene nanofluid. The findings of our study shows that the concentration of CNTs and their functionalization play a crucial role in improving the thermal conductivity of this biodegradable solvent

*18th International Congress on Thermal Analysis and Calorimetry, IITMadras, India,02-07 Sept. 2024*

# Investigation of component interaction in aqueous solution of nicotinic acid solutions in presence of L-Serine: volumetric, acoustical, viscometry and optical properties studies.

**B. R. BHOSALE[1]*, H.N. PAWAR[1], A. D. ARSULE[2], S.D. DEOSARKAR[1]**

[1]School of Chemical Sciences, Swami Ramanand Teerth Marathwada University Nanded 431606
(MS) India
*Corresponding author: bhosaleb700@gmail.com

**Keyword:** Ultrasonic Velocity, Optical properties, Volumetric, Transport properties, Molecular interactions.

The Experimental density (ρ), ultrasonic velocity (u), viscosity (η) and refractive index ($n_D$) of aqueous solutions of the vitamin $B_3$ (Nicotinic acid) have been measured in presence of amino acid L-serine at different temperatures (303.15K, 308.15K, 313.15K and 318.15K) at 1 atmospheric pressure .The density and ultrasonic velocity data has been utilised for the calculations of apparent molar volume( v2ϕ) and compatibilities ( ks2ϕ )of nicotinic acid. The linear dependence of apparent molar properties over the molal concentration of the vitamin B3 where predicted the Masson's and Gucker's relation respectively and corresponding partial molar properties namely, partial molar volume and compatibilities where determined. In addition to that the viscosity and refractive index of the studied system can be carried out. The result interpreted in terms of molecular interaction between solute-solute, solute-solvent and solute –co solute.

## References

[1] B.K.Chennuri, V Losetty, R. L. Gardas,J. Mol.liq.212(2015)444-450.
[2] S.D. Deosarkar , A.D. Arsule, R.T. Sawale, V.G. Pingle,J. of Mol. Liq.323 (2021) 114925.
[3] G. Ayranci, M. Sahin, E. Ayranci, J. Chem.Thermodyn. 39(2007)1620–1631

*18th International Congress on Thermal Analysis and Calorimetry, IITMadras, India,02-07 Sept. 2024*

---

# Determination of Critical Micelle Concentration (CMC) of Sodium Stearate Solution in Different Temperature

**<u>Brahamdeo Yadav</u>[a], Chandradip Kumar Yadav[b,c*], Manoj Adhikari, Rakesh Benedict[c], Yog Prakash Yadav, Neelam Shahi[c], Ajaya Bhattarai[*]**

[a] Suranarayan Stayanarayan Morbaita Yadav Campus, Tribhuvan University, Sirah, [b]*Amrit Science Campus, Tribhuvan University, Thamel,* [c]*CSIR- Institute of Minerals and Material Technology, Bhubaneswar, India,* [d] *Mahendra Morang Adarsh Multiple Campus, Tribhuvan University, Biratnagar, Nepal*

*Corresponding author: e-mail: l: bkajaya@ yahoo.com

**Keywords**: Surfactant, specific conductivity, polar, Critical Micelle Concentration

Surfactant is an organic compound having polar and nonpolar parts. specific conductivity of sodium stearate surfactant in double distilled water has been studied by conductometric method at three temperatures (298.15, 308. 15, 318.15) K. Critical Micelle Concentration (CMC) of sodium Stearate was determined at all temperatures. CMC is increases with an increase in temperature of the solution. FESEM image, EDX graph shows the purity of the sample. The percentage of elements present in sodium stearate surfactant has been explained by EDX data.

The percentage of C, O, Na, sodium stearate surfactant is 77, 14.2, 2.5 percent by weight.

*18th International Congress on Thermal Analysis and Calorimetry, IITMadras, India,02-07 Sept. 2024*

# Novel observation of Negative heat capacity and Fragility threshold in AgI-Ag$_2$O-MoO$_3$ glass

**B. TANUJIT***

Department of Science and Humanities, CHRIST University, Kengeri Campus, Kengeri, Bangalore - 560 074, Karnataka, India)
*Author: e-mail: tanujit.biswas@christuniversity.in

**Keywords**: Thermal analysis, Alternating Differential Scanning Calorimetry (ADSC), Negative heat capacity, glass.

ADSC (40°C-200°C) studies are performed on the $(AgI)_{75-x}$-$(Ag_2O)$-$(MoO_3)_x$ glasses for $20 \leq x \leq 37.5$. The total heat capacity, $C^* \approx C_{pPCR}$, where $C_{pPCR}$ is the in-phase, phase corrected reversing heat capacity, because other than melting, phase correction of $C^*$ is negligible [1]. Now, an abrupt change is observed in the sign of $C_{pPCR}$ at glass transition temperature, $T_g$ i.e. $C_{pPCR}(T_g)$. **Figure 1** shows that $T_g$ increases monotonically with the MoO$_3$ concentration but $C_{pPCR}(T_g)$ shifts from negative (Region I) to positive (Region II) almost abruptly at a threshold.

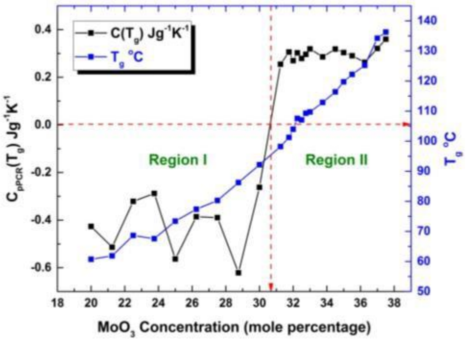


Fig. 1: $C_{pPCR}(T_g)$ ($Jg^{-1}K^{-1}$) and $T_g$°C vs. MoO$_3$ concentration (mole percentage)

A study on the effect of pressure on conductivity in this glass [2] suggests a model where the glass is composed of conductive clusters connected by less dense compressible material. Moreover, studies [3] on the thermodynamic behavior of nanoclusters where two different structural phases separated by free energy barrier suggest that such clusters can give rise to the negative slope in the caloric curve, causing negative heat capacity. Thus, it is inferred that experimentally obtained negative $C_{pPCR}$ is a reflection of a structural phase consisted of tissue and metallic clusters.

## References

**[1]** M. Reading et al., *Modulated-Temperature Differential Scanning Calorimetry*, Springer, **2006**.
[2] H. Senapati et al., *Effect of Pressure on the fast-ion conduction in AgI-Ag$_2$O-MoO$_3$ glasses*, Philosophical Magazine B, 47, 3, (**1983**), 291.
[3] K. Michaelian et al., *Critical Analysis of Negative Heat capacity in Nanoclusters*, European Physics Letter, 79, (**2007**) 43001.

# Climate Chamber-Assisted Oil-Bath Calorimetry for Accurate Specific Heat Determination of Lithium-Ion Cells

**FARAZ P. JUNAID[1,2,*] AAKASH SADAR[1], DIBAKAR RAKSHIT[1,*]**

[1]Department of Energy Science and Engineering, Indian Institute of Technology Delhi, New Delhi 110016, India.
[2] Mechanical Engineering Department, T.K.M. College of Engineering, Kollam, Kerala 691005, India
*Corresponding author: e-mail: dibakar@dese.iitd.ac.in, esz228279@iitd.ac.in

**Keywords**: climate chamber, specific heat, in-situ, lithium-ion cell, oil bath calorimetry.

Specific heat is a critical thermal property in the analysis of battery thermal management system [1]. For the in-situ measurement of the specific heat of a prismatic lithium-iron phosphate cell, a modified experimental methodology is adopted for the oil bath calorimetry to eliminate the heat losses to the surroundings from the calorimeter.

The adiabatic container filled with oil is placed inside a climate chamber. The chamber's temperature is continuously adjusted to match the inner surface temperature of the adiabatic container. This approach minimizes the temperature difference between the interior and exterior of the container, effectively creating near-adiabatic conditions. As a result, heat transfer is minimized, allowing for precise measurements of thermal interactions within the container. Applying the energy balance between the initial state and the state in which the battery and oil are in thermal equilibrium, the specific heat value of the battery was obtained as 1588.27 kJ/kg K. The initial temperature of the battery and oil was 43.5 and 30 °C, respectively. The system reached thermal equilibrium with a temperature of 40.9 °C at 5080 s as shown in Fig. 1.

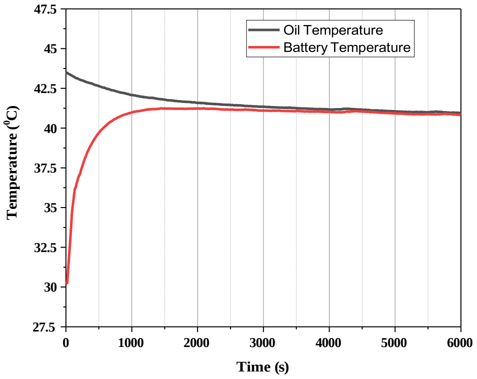


Fig. 1. Variation in battery and oil temperature with time inside the adiabatic chamber.

## References

[1] J. Shi, H. Zhang, H. Yu, Y. Xu, S. Xu, L. Sheng, X. Feng, X. Wang, Experimental determinations of thermophysical parameters for lithium-ion batteries: A systematic review, ETransportation 20 (2024). https://doi.org/10.1016/j.etran.2024.100321.

*18th International Congress on Thermal Analysis and Calorimetry, IITMadras, India,02-07 Sept. 2024*

# Volumetric and compressibility studies of antimycobacterial drug in aqueous and aqueous D-glucose solutions at various temperatures

**VANDANA S. SHENDE, ANUJA JAIN, SANGESH P. ZODAPE***
Department of Chemistry, Visvesvaraya National Institute of Technology (VNIT), Nagpur- 440 010, Maharashtra, India
*Corresponding author: e-mail: szodape@chm.vnit.ac.in, sangesh02@gmail.com

**Keyword:** D-glucose; apparent molar volume; apparent molar isentropic compressibility; Hepler constant

In the current research, we reported the density ($\rho$) and speed of sound ($u$) data of an antimycobacterial drug in aqueous binary solutions and aqueous ternary solutions comprising fixed concentration (0.06 and 0.1 $mol.kg^{-1}$) of D-glucose within the concentration range 0.01 to 0.15 $mol.kg^{-1}$ at different temperatures (293.15,298.15,303.15,308.15 and 313.15 K) and atmospheric pressure. The experimental ρ and u data were used to compute apparent molar volume of solute ($V\phi$) , limiting apparent molar volume of solute $V^0\phi$ , limiting apparent molar expansivity of solute $E^0\phi$ , thermal expansion coefficient ($\alpha$) , apparent molar compressibility of solute ($KS,\phi$) , limiting apparent molar compressibility of solute( KS, $^0\phi$ and hydration number ($nh$). It is noted that $E^0\phi$ in water goes through a minimum as a function of temperature. The values of transfer partial molar volume $\Delta tr^0V\phi$ and transfer partial molar compressibility $\Delta tr^0K\phi$ from aqueous-to aqueous D-glucose solutions are estimated. The outcomes are examined and deliberated on the basis of interactions occurs in binary and ternary mixtures.

## References

[1] V. S. Shende, U. R. Pratap, A.V.Wankhade, and S. P. Zodape, J. Mol. Liq. 321 (2021) 114755.
[2] A.Jain, V. S. Shende, D. V. Kawadkar, U. R. Pratap, A.V.Wankhade, and S. P. Zodape, J. Chem. Thermodyn. 162 (2021) 106561
[3] V. S. Shende, U. R. Pratap, A.V.Wankhade, and S. P. Zodape, J. Molecular Liq. 337 (2021) 116580.
[4] T. S. Banipal, H. Singh, and P. Banipal, J. Chem. Eng. Data, 55 (9) (2010) 3872.

*18th International Congress on Thermal Analysis and Calorimetry, IITMadras, India,02-07 Sept. 2024*

# Investigation of volumetric, optical and transfer properties of ascorbic acid with different cosolutes at 303.15 K

**R. V. DUDHATE, H. N. PAWAR, A. D. ARSULE, AND S. D. DEOSARKAR***

School of Chemical Sciences, Swami Ramanand Teerth Marathwada University, Nanded 431 606 (MS) India
*Corresponding author: e-mail: sandeo24@srtmun.ac.in

**Keywords**: viscosity, molecular interaction, optical properties

Present work reports the molecular interactions between ascorbic acid solute (0.05 to 0.5) mol·kg$^{-1}$ and sucrose/β-cyclodextrine/potassium chloride in aqueous solution at temperature 303.15 K and atmospheric pressure. For this, the density data are utilized to determine apparent molar volume ($V_{\varphi}$), limiting apparent molar volume ($V^{o}_{\varphi}$) of solute. The viscosity measurements were employed to calculate relative viscosity and subsequently the viscosity $A$ and $B$ coefficients of aqueous solutions. The surface tension and refractive index of studied systems have also been measured. The results obtained have been interpreted in term of solute-solvent and solute-solute interactions and shows the structure making/breaking ability of ascorbic acid in different aqueous-cosolute solutions.

**References**

[1]B.K.Chennuri, V Losetty, R. L. Gardas, *J. Mol.liq.*212 **(2015)**444-450.
[2] G. Ayranci, M. Sahin, E. Ayranci, *J. Chem. Thermodyn*. 39 **(2007)**1620–1631.
[3] S.D. Deosarkar, A.D. Arsule, R.T. Sawale, V.G. Pingle, *J. of Mol. Liq.*323 (**2021)** 114925.

*18th International Congress on Thermal Analysis and Calorimetry, IITMadras, India,02-07 Sept. 2024*

# Density and Utraacoustic Properties of Antibacterial Pyridoxine Hydrochloride and Neomycin Sulphate Drugs in Aqueous Carbamide Solutions at Different Temperatures

**M. P. PAWAR[1], S. D. DEOSARKAR[2], H. N. PAWAR[2], R.V. DUDHATE[2] & A. D. ARSULE[*]**
[1]School of Chemical Sciences S R T M University, Nanded (MS) India-431606
[2]School of Chemical Sciences S R T M University, Nanded (MS) India-431606
[*]Department of Chemistry, Madhavrao Patil ACS College Palam, Parbhani (MS) India-431720
Corresponding author e-mail: atmaram0007@gmail.com

**Keywords**: Thermodynamic properties, molecular interactions, drugs solution,

The experimental density and ultrasonic velocities values of pyridoxine hydrochloride and neomycin sulphate drugs in aqueous urea (carbamide) solutions have been measured as function of drugs concentration at different temperatures ($T$= 303.15, 308.15 and 313.15) K. From these experimental values we have computed derived thermodynamic properties such as acoustic impedance ( $Z$ ), isentropic compressibility ( $K_s$ ), intermolecular free length ( $L_f$ ) and relative association ( $R_A$ ). We have investigate how the drug is affected by co-solutes as well as drugs behaviour in water and water + urea system can be studied to explore the different types of molecular interactions.

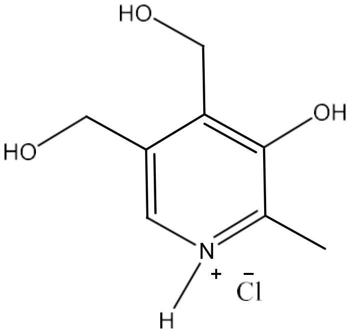


Fig. 1: Chemical structure Pyridoxine hydrochloride

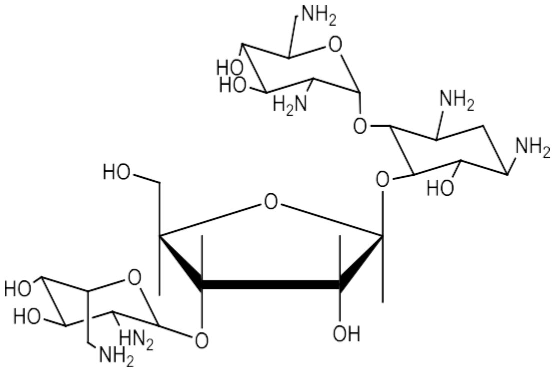


Fig. 2: Chemical Structure of Neomycin sulphate

## References

[1] N. Ahuja, O. P. Katare and B. Singh. *Eur. J. Pharm. Biopharm,* 65 (**2007**) 26.
[2] N. Okulik and A. H. Jubert. *J. Mol. Struct. Theochem,* 769 (**2006**) 135.
[3] S. Shrikant, T. Joshi, M. Aminabhavi and S.S. Shukla. *J. Chem. Eng. Data,* 35 (**1990**) 187.

*18th International Congress on Thermal Analysis and Calorimetry, IITMadras, India,02-07 Sept. 2024*

# Partial molar volumes, compressibilities and viscosities of Ranitidine Hydrochloride in aqueous-NaCl/sucrose solutions at 303.15 K

**H. N. PAWAR, R. V. DUDHATE, A. D. ARSULE, P. D. TAWDE AND S. D. DEOSARKAR***

School of Chemical Sciences, Swami Ramanand Teerth Marathwada University, Nanded 431 606 (MS) India
*Corresponding author: e-mail: sandeo24@srtmun.ac.in

**Keywords**: density, ultrasonic velocity, molecular interactions, drug solution

The densities, ultrasonic velocities and viscosities of antacid drug ranitidine hydrochloride in aqueous-NaCl/sucrose solutions were measured as a function of concentration of drug and cosolutes at 303.15 K. The apparent molar volumes and compressibilities of ranitidine were calculated from density and ultrasonic velocity data and calculated apparent molar properties were used to determine partial molar volumes and compressibilities of ranitidine using standard relations. Also, the relative viscosities of solutions were evaluated in terms of viscosity *B*-coefficients. The effect of added cosolutes on hydration behavior of solute drug has been evaluated through studied properties in terms of solute-solvent and solute-cosolute interactions. Results showed structure making nature of NaCl and sucrose in aqueous-ranitidine hydrochloride solutions.

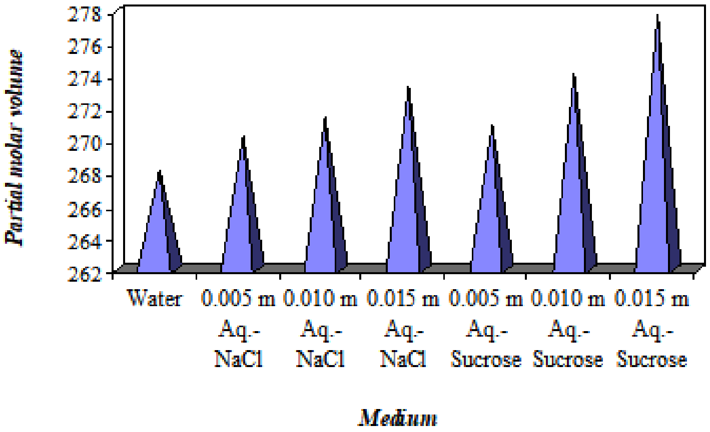


Fig. 1 : Partial molar volumes of ranitidine hydrochloride in different aqueous medium at 303.15 K

**References**
[1] ] K. K. Athira, Ramesh L. Gardas, *Journal of Molecular Liquids*,389**(2023)**122858.
[2] S.S. Dhondge, S.P. zodape, D.V. Parwate, *Journal of chemical Thermodynamics*,48**(2012)**207-212.
[3]S.D. Deosarkar , R.T. Sawale and R.V. Pinjari, *Chemical Physics Impact*, 08**(2024)**100580.

**T1- PP 11**

# Thermophysical properties of a newly synthesized cationic surfactant

**JULFIKAR HASSAN MONDAL[1], MD. SAYEM ALAM[1,2]***

[1] Department of Polymer Science and Technology, CSIR-Central Leather Research Institute, Chennai-600020, India.
[2]*Chemical Sciences, Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, Uttar Pradesh 201 002, India.*

*Corresponding author: e-mail: *sayem@clri.res.in*,

**Keywords**: Surfactant, Synthesis, Characterization, Micelle, Thermodynamics

Cationic surfactants represent a crucial class of amphiphilic compounds with a positively charged hydrophilic head group. Understanding the behaviour of cationic surfactants is essential for optimizing their applications.

We have synthesized a new cationic surfactant aimed at enhancing interfacial activity in various applications. Characterization techniques including FT-IR, NMR and ESI mass spectra were employed to assess the purity of the synthesized surfactant.

Critical micelle concentrations (CMC) of mixed surfactant-hydrotrope systems were determined by conductometric technique. CMC values of surfactant-hydrotrope decrease with increasing hydrotrope concentration. Interactions between hydrotrope and surfactant are synergistic in nature. We also deduced thermodynamic parameters of micellization (viz., $\Delta G^0_m$, $\Delta H^0_m$, $\Delta S^0_m$). The effect of hydrotrope and temperature on different thermophysical properties has been discussed. Experimental techniques like FT-IR and NMR were employed to reveal the non-covalent interactions of mixed surfactant-hydrotrope systems. Further investigations will focus on optimizing formulation and exploring specific applications to harness its full potential in practical scenarios.

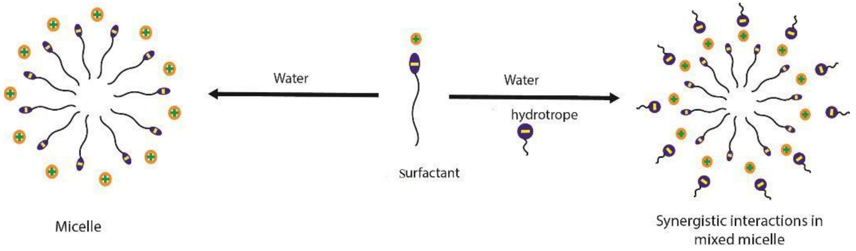


Fig. 1: Schematic presentation of surfactant self-assembly.

**References**

[1] R. A. Gonçalves, K. Holmberg and B. Lindman, *Journal of Molecular Liquids*, 375 (**2023**) 121335.

**T1- PP 12**

# Thermodynamic, transport and structural studies of Imidazolium Ionic liquids and Molecular solvents mixtures at (298.15 to 323.15) K and 0.1 MPa

**MALIK RAIHAN AHMAD[1], RIYAZUDDEEN[2*]**

[1,2] Department of Chemistry, Aligarh Muslim University, Aligarh 202002, UP, India
*Corresponding author: e-mail: rz1@rediffmail.com

**Keywords**: Imidazolium Ionic Liquids, Molecular solvents, Thermodynamic Properties, Transport Properties, Density functional theory, FT-IR

The experimental thermophysical properties, including densities (ρ), speeds of sounds ($u$), and dynamic viscosities (η), of binary mixtures, 1-butyl-3-methylimidazolium trifluoromethane sulfonate and 2-methoxyethanol / 2-propoxyethanol have been measured experimentally at temperatures (298.15,303.15, 308.15K, 313.15, 318.15, 323.15) K and at atmospheric pressure. Excess molar volumes ($V^E$), isentropic compressibility deviations ($\Delta\kappa_S$), viscosity deviations ($\Delta\eta$), Gibbs energies of activation, ($\Delta G^*$) and excess Gibbs free energies of activation, ($\Delta G^{*E}$) values are computed using values of pure Ionic liquid / molecular solvent and of their binary mixtures. This study focuses on how composition and temperature determine the strength of ion-ion, ion-dipole, and dipole-dipole interactions in the mixtures. In order to understand the model fitting, the derived/excess properties have been fitted to the Redlich-Kister polynomial equation. The excess molar volume has also been correlated with the PFP theory to justify the obtained results. The impact of molecular solvents on interactions is accounted for by the DFT study, which examines the interactions between the ionic liquid and the surrounding molecular solvents, both within and between the ions, providing detailed insights into interactions within isolated ILs and their binary mixture [1-4].

.

## References

[1] J. Safarov, A. Guluzade *J Chem Eng Data*, 64 (**2019)** 2247.
[2] U. Fatima, Riayzuddeen. *J Solution Chem*. 45, (**2018**), 1077.
[3] L., Zhao, F., Zhang, *J Chem Eng Data, 53,* (**2008**), 2408.
[4] E. González, Á. Domínguez, J *Chem Eng Data,* 57, (**2012**), 2165.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Enhanced Micellization and Structural Transformation in Morpholinium-Based Ionic Liquids with Aromatic Counterions

**SANJAY H. PANJABI[1]*, RAVI VIRADIYA[1], V K ASWAL[2]**

[1]Chemical Sciences Department, P D Patel Institute of Applied Sciences, Charotar University of Science and Technology, Changa, Gujarat, India -388421
[2]Solid State Physics Division, Bhabha Atomic Research Center (BARC), Mumbai 400085, India;

**Keywords**: Surface-active ionic liquids, Aromatic counterions, Micellization, Small-angle neutron scattering

In this study, we synthesized two novel morpholinium-based surface-active ionic liquids (SAILs) with aromatic counterions: n-dodecyl-n-methylmorpholinium salicylate ([$C_{12}$mmor][Sal]) and n-dodecyl-n-methylmorpholinium 3-hydroxy-2-naphthoate ([$C_{12}$mmor][3-H-2-n]). We systematically explored their aggregation behavior in aqueous solutions using various analytical techniques, including electrical conductivity, small-angle neutron scattering (SANS), surface tension measurements, and UV-Vis spectroscopy. Our findings revealed that incorporating aromatic counterions enhances the micellization properties compared to conventional halogenated SAILs such as [$C_{12}$mmor][Br]. SANS analysis showed a structural transformation from prolate ellipsoidal micelles to large unilamellar vesicles when the counterion was changed from salicylate to 3-hydroxy-2-naphthoate. Thermogravimetric analysis (TGA) was employed to assess the thermal stability of the synthesized SAILs. The TGA results indicated high thermal stability for both [C12mmor][Sal] and [C12mmor][3-h-2-n], which is crucial for their potential applications in various high-temperature processes. Additionally, we observed that increasing the concentration of [$C_{12}$mmor][Sal] resulted in a lower aggregation number. We present comprehensive thermodynamic, micellar, and interfacial parameters, including the degree of counterion binding (β), critical micelle concentration (CMC), minimum area per molecule ($A_{min}$), surface excess concentration ($\Gamma_{max}$), standard Gibbs free energy of adsorption ($\Delta G_{ad}°$), aggregation number (Nagg), standard Gibbs free energy of micellization ($\Delta G_m°$), standard enthalpy of micelle formation ($\Delta H_m°$), and standard entropy of micellization ($\Delta S_m°$). This study underscores the potential of aromatic counterions in morpholinium-based SAILs to improve micellization properties, offering new insights into the design of efficient and environmentally friendly surfactants. The results have significant implications for various applications, including catalysis, drug delivery, and materials science.

**T1- PP 14**

# Influence of PbO on thermal behaviour of boro-tellurite glasses

**Nibedita Samanta[1*], Abhiram Senapati, Hrudananda Jena[1,2]**

[1]Materials Chemistry and Metal Fuel Cycle Group, IGCAR, Tamilnadu, 603102, India
[2] Homi bhabha National Institute, Anushakti Nagar, Mumbai 400094,India
*Corresponding author: nibedita@igcar.gov.in

**Keywords**: tellurite glass, thermal stability, DSC, glass transition temperature

Tellurite glasses are of great scientific interest in optoelectronic and radiation field due to their interesting physical and optical characteristics. Tellurite glasses doped with PbO is a potential candidate as radiation protection material from gamma rays and neutrons [1]. In the present study, thermal properties of boro-telluride glasses are studied with varying concentration of PbO.

The glasses were prepared using conventional melt quenching method with nominal composition of $x$PbO-40$B_2O_3$-(60-$x$)$TeO_2$ where $x$ = 10, 15 and 20 mol% and assigned as 10PbBTe, 15PbBTe and 20 PbBTe respectively.

The XRD pattern of the glass samples are presented in Fig. 1 and it shows broad band around 20-30 degree reflecting the amorphous nature of glasses. Thermal stability of the glasses were studied by Differential Scanning calorimetry (DSC). Glass transition temperature ($T_g$) were obtained from the DSC curves and shown in Fig. 2 as a function of composition of PbO. It shows that $T_g$ values decreases from 396 to 383ºC with the increased amount of PbO from 10-25 mol%. This may be due to the degradation of structure as the substitution of PbO in the structure breaks the group of bridging oxygens inside the tellurite glass structure. Hence addition of PbO decreases the $T_g$ of the boro-tellurite glasses.

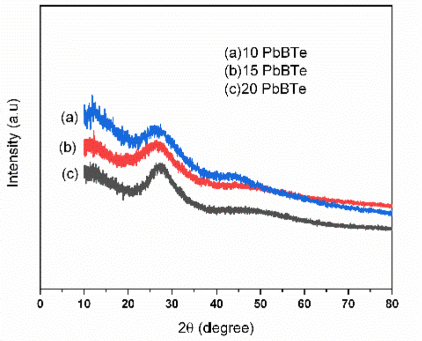


Fig. 1: XRD pattern of Pb-boro-tellurite glasses

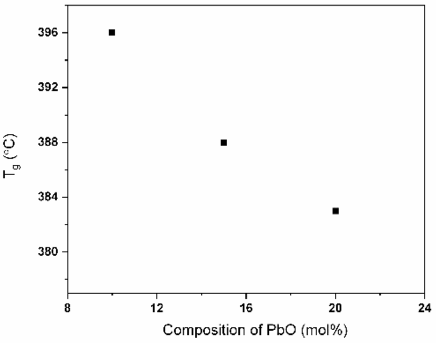


Fig. 2: Variation of $T_g$ with the composition of PbO

## Reference

[1] Recep Kurtulus, Taner Kavas, Esra Kavaz, Ghada AlMisned, H.O.tekin, *Ceram. Int.* 49 **(2023)** 23189.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Biophysical Study to Investigate the Interaction of some of aminoglycosides with *Mycobacterium tuberculosis* G-quadruplex DNA

**ANUPAMA RAI, NIKI SWETA JHA***

Department of Chemistry, National Institute of Technology, Patna-800005, India
E-mail: nikij@nitp.ac.in

**Keywords**: Aminoglycosides, Mycobacterium Tuberculosis, G-quadruplex DNA, Biophysical, Calorimetric study

Aminoglycosides are known to stabilize parallel G-quadruplex DNA *via* non-covalent interactions [1]. In case of bacteria as well targeting the G-quadruplex motifs by selective small molecule has been known to reduce the survival and virulence of the bacteria [2-4]. Here, we are reporting interaction of two aminoglycosides *i.e.,* streptomycin and neomycin with *Mycobacterium tuberculosis* G-quadruplex DNA *i.e.,* espK and cyp51 through biophysical, and calorimetric methods. These G4 DNA sequence (espK and cyp51) is involved in pathways that are responsible for virulence determination of bacteria inside the host cell and its survival by maintaining membrane fluidity. Affinity of these aminoglycosides for G-quadruplex binding has been screened by absorption spectroscopy, fluorescence spectroscopy, circular dichroism (CD) spectroscopy, thermal melting, and isothermal titration calorimetry (ITC) experiments, respectively. The spectral studies shows that both the ligand have affinity with espK and cyp51 G-quadruplex DNA, but their mode of bindings is different. The experiments evidence shows the stabilization of espK and cyp51 in presence of neomycin, while streptomycin destabilizes the bacterial DNA. The binding isotherms of neomycin with both G4 DNA were exothermic with 8.13 x $10^6$ $M^{-1}$ binding affinity for espK and 9.90 x $10^6$ $M^{-1}$ for cyp51 for single binding site at 50 mM KCl.

**References**

(1) Ranjan, N.; Arya, D. P. Parallel G-Quadruplex Recognition by Neomycin. *Front Chem* **2023**, 11.
(2) Endoh, T.; Kawasaki, Y.; Sugimoto, N. Suppression of Gene Expression by G-Quadruplexes in Open Reading Frames Depends on G-Quadruplex Stability. *Angewandte Chemie International Edition* **2013**, 52 (21), 5522–5526.
(3) Mishra, S. K.; Shankar, U.; Jain, N.; Sikri, K.; Tyagi, J. S.; Sharma, T. K.; Mergny, J.-L.; Kumar, A. Characterization of G-Quadruplex Motifs in EspB, EspK, and Cyp51 Genes of Mycobacterium Tuberculosis as Potential Drug Targets. *Mol Ther Nucleic Acids* **2019**, 16, 698–706
(4) Yadav, P.; Kim, N.; Kumari, M.; Verma, S.; Sharma, T. K.; Yadav, V.; Kumar, A. G-Quadruplex Structures in Bacteria: Biological Relevance and Potential as an Antimicrobial Target. J Bacteriol 2021, 203 (13).

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Investigation of Molecular Interactions by Volumetric, Ultrasonic, Spectral and Computational Studies in Selected Binary Liquid Mixtures of 2-Chloro Ethanol over the Temperature Range 298.15 - 323.15 K

**D. BALA KARUNA KUMAR[1*], SK. N. SHAREEF[1] P. SUGANDHA KUMAR[2], O. BASWANTH[3]**

[1]Department of Chemistry, Andhra Loyola College, Vijayawada, Andhra Pradesh, India-520 008
[2]Department of Chemistry, ALIET, Vijayawada, Andhra Pradesh, India-520 008
[3]School of Mathematics and Natural Sciences, Chanakya University, Devanahalli, Bangaluru -562165
*Corresponding author: dbkkumar123@gmail.com

**Keywords**: Density, ultrasonic speed, Redlich–Kister polynomial, FT-IR, Molecular interaction

Liquid mixtures are indispensable in almost all industries and the knowledge of intermolecular interactions plays a crucial role in modulating their physico-chemical properties [1]. This paper is a part of our continuing and systematic investigation of binary mixtures from thermodynamic, acoustic and spectroscopic aspects [2-4]. In the present study the densities, sound speeds and refractive indices are experimentally determined for pure liquids 2-Chloroethanol (2-CLE), N-methyl aniline (NMA), N,N-dimethyl aniline (DMA) and N,N-diethyl aniline (DEA) and their binary mixtures containing 2-CLE as a common component at atmospheric pressure as a function of composition of 2-CLE in the temperature range 298.15 - 323.15 K. From the experimental data excess molar volumes, excess partial molar volumes, excess icentropic compressibilities and deviations in ultrasonic speed are computed and fitted to a Redlich–Kister type equation. An attempt is made to use necessary FT-IR spectral analysis of the binary mixtures to understand the interactions present and to correlate them with thermodynamic findings. Also, Gaussian-16 molecular modeling software is used to perform computational studies to examine the experimental results with computational Analysis. DFT calculations are also performed to get the estimate of interaction energies between the component molecules of the studied mixtures.

## References

[1] D.B.K. Kumar, K.R. Reddy, G. Srinivasarao, G.V. Ramarao, C. Rambabu, *J. Mol. Liq.*, 174 **(2012)** 100–111.
[2] D.B.K. Kumar, K.R. Reddy, G. Srinivasarao, P.V.S. Sairam, C. Rambabu, *J. Mol. Liq.*, 199 **(2014)** 352-363.
[3] D.B.K. Kumar, T.S. Krishna, O, Baswanth, C.V. Pramod, G.S. Rao, *J. Mol. Liq.*, 337 **(2021)** 116449
[4] T. Ankaiah, K. Srinivas, Sk. N. Shareef, D.B.K. Kumar, et al, *J. Chem. Eng. Data* 69 **(2024)** 1423-1447

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# A study on thermophysical, physiochemical, and surfaces properties of fatliquors

**Aswini Annadurai** [1], **Md. Sayem Alam** [1, 2,*]

[1]Council of Scientific and Industrial Research (CSIR) — Central Leather Research Institute (CLRI), Polymer Science & Technology Unit, Advanced Materials Laboratory, Chennai 600020, India,
[2]Chemical Science, Academy of Scientific and Innovative Research (AcSIR ), Ghaziabad, Uttar Pradesh - 201 002, India.
*E-mail: sayemalam@gmail.com, sayem@clri.res.in

**Keywords**: Fatliquors, Leather lubricant, Emulsion, Thermal analysis, Particle size

Fatliquoring is an important post-tanning operation that is carried out on tanned leather using oils, fats, or greases in emulsion form to make soft leather, and improve the physical characteristics of the finished products. For making better leather and eco-friendly, it is very important to know the physicochemical properties of the fatliquors. To the best of our knowledge, the physicochemical characteristics of the majority of commercial fatliquors are unknown. Therefore, this research aims to investigate the physicochemical properties of these commercial fatliquors (viz., phospholipid, silicone, paraffin, and synthetic oil-based, etc.) by different techniques (viz., conductometric, viscometric, DSC, and TGA (thermal behaviours), microscopic, particle size (mean/average), the zeta potential, etc.). The data presented in this study will help to make or formulate fatliquors that could help to improve the quality of the leather according to the market demands. The information in this work's findings will assist in choosing a reasonable fatliquor for planning a fatliquoring manner for improving 'quality leather'.

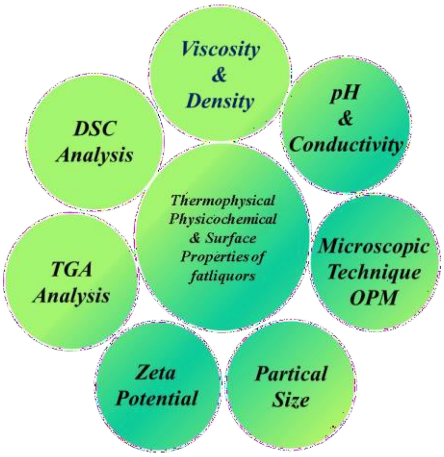


Fig. 1: Thermo physical, physiochemical, and surfaces properties of fatliquors

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermophysical properties of thermal energy storage medium for battery cooling: Thermophysical properties of 2,5-dimethyl-2,5-hexanediol hydrates

**I. MITSUI[1]*, R. OHMURA**

[1]Department of Mechanical Engineering, Keio University, Yokohama 223-8522, Japan

**Keywords**: hydrate, energy storage, phase change materials, phase equilibrium

The renewable energy has the potential to solve environmental problems. The goal of renewable energy is to achieve stable generation and supply. Energy storage system (ESS) enable supply of renewable energy. There are several systems for ESS, of which lithium-ion batteries are the most widespread. However, the weak point of the lithium-ion battery is heating due to charging and discharging. The ideal battery operating temperature is about 40 ℃ . It is necessary to cool the battery and conventional cooling methods include forced convection cooling and water cooling. Using 2,5-dimethyl-2,5-hexanediol (DM-HDO) hydrate as phase change material (PCM) is proposed as a new method. The hydrate has a large dissociation heat and will form and dissociate at approximatery 40 ℃ under atmosphere pressure conditions. Battery cooling which uses DM-HDO hydrate would have enough performance regarding that stability of heat transfer. To adapt DM-HDO to battery cooling, it is necessary to clarify the changes in physical properties as the concentration of the aqueous solution is varied.

In this study, the equilibrium temperature and dissociation heats were measured. The equilibrium temperature was measured by visual observation, the dissociation heats were measured by DSC. The range of aqueous solution concentration was 0.40 to 0.52 in mass fraction. The highest equilibrium temperature was 38.3 ℃, the dissociation heat was 165.3 kJ/kg at the mass fraction of 0.50.

Table 1: The equilibrium temperature and dissociation heat of DM-HDO hydrate

| Mass fraction, $w$ | Equilibrium temperature, $T_{\mathrm{eq}}$ /℃ | Dissociation heat, $\Delta H$ /kJ · kg$^{-1}$ |
|---|---|---|
| 0.41 | 37.6 | 123.2 |
| 0.46 | 38.1 | 146.3 |
| 0.47 | 38.0 | 147.6 |
| 0.50 | 38.3 | 165.3 |

**References**

[1] B. Shabani, M. Biju, *Energies.* 8 (2015) 10153-10177

[2] Goates, J. R., Bevan Ott, J., Woolley, E. M., & Priest, J. G. (1982). *J. Chem. SOC., Faraday Trans.* 1 (Vol. 78).

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Impact of Carboxylate Anion Chain Length and Temperature on Physicochemical Properties of Butyrolactam-based protic Ionic Liquids

**Bignya Rani Dash, Ramesh L. Gardas*, Ashok Kumar Mishra***
Department of Chemistry, Indian Institute of Technology Madras, Chennai 600036, INDIA
*Corresponding author: e-mail(s): mishra@iitm.ac.in, gardas@iitm.ac.in

**Keywords**: protic ionic liquids, volumetric properties, DSC, microheterogeneity

Ionic liquids (ILs), composed of cations and anions, possess negligible vapor pressure, high thermal stability and most of them exist as a liquid at room temperature, known as room temperature Ionic Liquids (RTILs).[1] Understanding both physicochemical properties and molecular-level heterogeneity of neat ILs is essential for better utilization in specific applications. The lactam-cation-based ILs have a relatively lower cost, lower toxicity, lower viscosity and comparable ion conductivity and heat storage density. They have wide applicable perspectives for fuel cell devices, thermal transfer fluids [2,3]. Herein, we have synthesized five carboxylates functionalised butyrolactam-based protic ionic liquids (PILs) by varying alkyl chain length of anions. The thermal stabilities of ILs were investigated by thermogravimetric analysis (TGA), while phase transition is measured by using differential scanning calorimetry (DSC). Various physicochemical properties such as density (ρ), viscosity (η), ionic conductivity (σ), and refractive index ($n_D$) were measured as a function of temperature from (293.15 to 333.15) K at atmospheric pressure. The experimental values of the viscosity and ionic conductivity were fitted well with the Vogel-Tammann-Fulcher (VTF) equation and Arrhenius equations [4]. Further, clear red-shift of the emission with an increased excitation wavelength was seen for five neat ILs. Subsequently, we have also shed light on inherent microheterogeneity within these ionic liquids through an microviscosity study by employing the Perrin equation [5]. The experimental results revealed the impact of structure variant on the transport properties such as viscosity and ionic conductivity and these insights help to design ionic liquids with desired applications.

**References**

[1] M. Dzida, E. Zorębski, M. Zorębski, M. Żarska, M. Geppert-Rybczyńska, M. Chorążewski, J. Jacquemin, I. Cibulka. Chemical Reviews, 117 (**2017**) 3883–3929.
[2] Z. Du, Z. Li, S. Guo, J. Zhang, L. Zhu, Y. Deng. Journal of Physical Chemistry B, 109 (**2005**) 19542–19546.
[3] P.K. Chhotaray, S. Jella, R.L. Gardas. Journal of Chemical Thermodynamics, 74 (**2014**) 255–262.
[4] R.L. Gardas, J.A.P. Coutinho, AIChE Journal 55 (**2009**) 1274–1290.
[5] B.R. Dash, R.L. Gardas, A.K. Mishra. Physical Chemistry Chemical Physics, 26 (**2024**) 13350 13363.

# The effects of natural environmental storage on the aging rate and thermal hazard characteristics of firecrackers

Chu-Yuan Yang[1], Wei-Chun Chen[2, *], Chi-Min Shu[1,3,*]
[1]Department of Safety, Health, and Environmental Engineering, YunTech, 123, University Rd., Sec. 3, Douliou 64002, Yunlin, Taiwan, ROC
[2]Bachelor Program in Industrial Technology, YunTech, 123, University Rd., Sec. 3, Douliou 64002, Yunlin, Taiwan, ROC
[3] Department and Graduate School of Safety, Health, and Environmental Engineering, YunTech., 123, University Rd., Sec. 3, Douliou, Yunlin, 64002, Taiwan, ROC
*Corresponding author: e-mail: chenwchun@gemail.yuntech.edu.tw and shucm@yuntech.edu.tw

**Keywords**: Explosion-like fireworks, aging phenomenon, simultaneous thermogravimetric analyzer, apparent activation energy, thermal stability

This study will provide an in-depth understanding of the impact of explosion-like fireworks on the hazardous properties of gunpowder compared with traditional firecrackers and environmentally friendly firecrackers stored in a normal room temperature environment for years and aging, using field emission scanning electron microscope (FE-SEM) and X-Ray photoelectron spectroscopy (XPS) observe the signs of aging caused by the influence of storage time on the sample microstructure and elements, it can be seen from the microscopic surface that firecrackers that have been stored for a long time have cracks and oxides due to oxidation and aging., then use simultaneous thermogravimetric analysis (STA) and advanced thermal analysis software to obtain thermal hazard parameters and calculate apparent activation energy. The difference in mass loss of traditional firecrackers in STA between 2005 and 2022 is significant, with a difference of 9.876%. The difference in quality loss of environmentally friendly firecrackers between 2012 and 2022 is less obvious, the difference is only 1.115%, showing that the aging of traditional firecrackers reduces thermal stability more seriously.

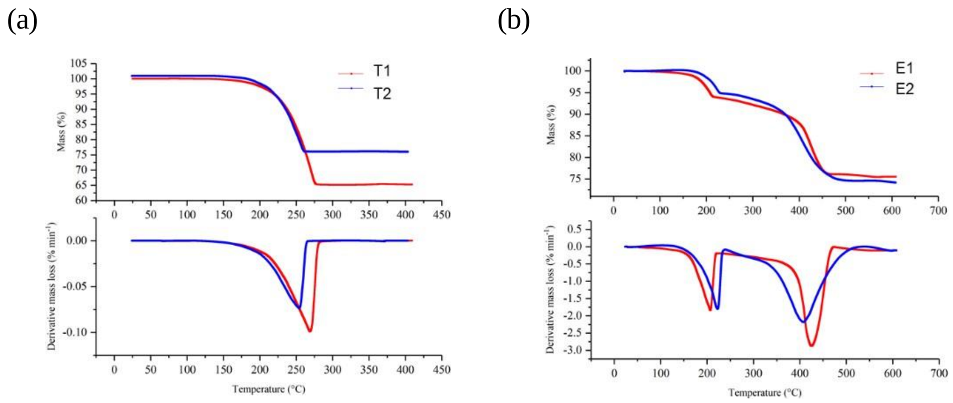


Fig. 1: The results of TG and DTG (a) traditional firecrackers; (b) environmentally friendly firecrackers

# Effects of adding various ionic liquids on the inflammability and thermal stability of industrial oils

Yu-Cheng Lin[1], Wei-Cheng Lin[2], Yi-Chun Yu[3], Chen-Rui Cao[4], Chi-Min Shu[2,3,*]
[1] Department of Safety, Health, and Environmental Engineering, YunTech, 123, University Rd., Sec. 3, Douliou, Yunlin 64002, Taiwan, ROC
[2] Centre for Process Safety and Industrial Disaster Prevention, YunTech, 123, University Rd., Sec. 3, Douliou, Yunlin 64002, Taiwan, ROC
[3] Department and Graduate School of Safety, Health, and Environmental Engineering, YunTech., 123, University Rd., Sec. 3, Douliou, Yunlin, 64002, Taiwan, ROC
[4] Graduate School of Engineering Science and Technology, National Yunlin University of Science and Technology, YunTech., 123, University Rd., Sec. 3, Douliou, Yunlin, 64002, Taiwan, ROC
*Corresponding author: e-mail: shucm@yuntech.edu.tw

**Keywords**: Boron-containing based ILs, Flame retardancy, Combustion, Phosphorus-containing based ILs, Fire protection

This study investigated the effects of incorporating phosphorus-containing based and boron-based ionic liquids (ILs), including 1-butyl-3-methylimidazolium dibutyl phosphate ([Bmim][DBP]), 1-butyl-3-methylimidazolium hexafluorophosphate ([Bmim][$PF_6$]), and 1-butyl-3-methylimidazolium acetate ([Bmim][$BF_4$]), on the flame retardancy and thermal stability of cutting oils and engine oils. These findings suggest that boron-based ILs could enhance high-temperature resistance and reduce heat release during combustion. Phosphorus-containing based ILs could form a protective carbon layer, thereby improving fire protection. Additionally, different ILs had varying effects on exothermic changes and thermal stability in industrial oils, with [Bmim][DBP] showing the most significant improvement.

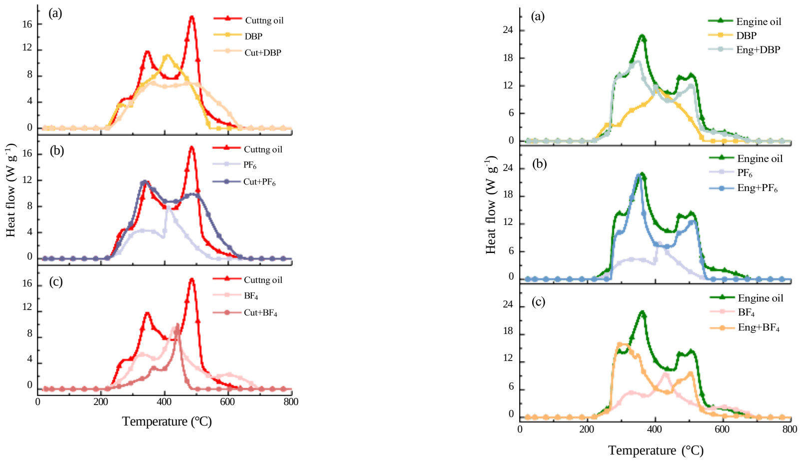


Fig. 1 : Heat flow versus temperature diagram of ILs, cutting, engine oils, and blended oils (a) [Bmim][DBP], (b) [Bmim][$PF_6$], (c) [Bmim][$BF_4$].

# Thermo physical study on binary mixtures of Furfural and *n*-butyl acetate or isobutyl acetate or tert-butyl acetate at 298.15, 303.15 and 308.15 K

**AARZOO[1]*, GYAN PRAKASH DUBEY[2]**

[1]Affiliation (Resreach Scholar)
[2] Department of Chemistry, Kurukshetra University, Kurukshetra 136119, India
*Corresponding author: e-mail: aarzooahuja655@gmail.com

**Keywords**: Furfural, Acetates, Excess molar volume, Excess/deviation properties, Redlich-Kister equation.

This paper presents the density ($\rho$), speed of sound ($u$) and viscosity ($\eta$) for furfural (FA), butyl acetate (BA), isobutyl acetate (IBA) and tert-butyl acetate (TBA) along with their binary mixtures containing furfural as a common component. These measurements were conducted at temperatures of 298.15 K, 303.15 K and 308.15 K covering the entire composition range. The obtained experimental data for density, speed of sound and viscosity were utilized in computing excess molar volume ($V_m^E$), excess molar isentropic compressibility ($\Delta K_{S,m}^E$), excess speed of sound ($u^E$), viscosity deviation ($\Delta\eta$), excess Gibb's free energy of activation for viscous flow ($\Delta G^{*E}$) and partial molar volume ($\bar{V}_{m,i}$). The fluctuations noted in these properties are influenced by composition and temperature. These variations are analyzed in relation to the molecular interactions arising from physical and chemical effects between the dissimilar molecules within the binary mixtures. Particularly, these properties including excess functions demonstrate significant sensitivity to intermolecular interactions within liquid mixtures. Furthermore, these excess functions and deviations have been correlated using a Redlich–Kister type polynomial equation through the method of least squares to estimate the binary coefficients and standard errors.

**References**

[1] M. Nduli, N. Deenadayalu. J. Mol. Liq. 241 (2017) 407-421.
[2] Z. C. Zhang, Wiley Interdiscip. Rev.: Energy Environ. 2 (2013) 655-672.
[3] L. Lomba, B. Giner, E. Zuriaga, J. Moya, C. Lafuente, J. Chem. Thermodyn. 66 (2013)131-136.
[4] W. P. Tai, H. Y. Lee, M. J. Lee, Fluid Phase. Equilib. 384 (2014) 134-142.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Experimental, theoretical and spectroscopic analysis of molecular interactions in binary liquid mixtures comprising 4-methyl-2-pentanol + $C_mH_{2m+1}OCH_2CH_2OH$ (m = 2,3,4) at different temperatures

**RACHANA SINGH, GYAN PRAKASH DUBEY***

Department of Chemistry, Kurukshetra University, Kurukshetra-136119, Haryana, India
* Corresponding author: e-mail: gyan.dubey@rediffmail.com

**Keywords:** excess molar volume, intermolecular interactions, structural effects, viscosity models, FT-IR

**Abstract:** In present communication we report the experimental values of density ($\rho$), viscosity ($\eta$) and speed of sound ($u$) of binary combinations of 4-methyl-2-pentanol with 2-ethoxyethanol, 2-propoxyethanol and 2-butoxyethanol at T = (298.15, 303.15 and 308.15) K. The excess and deviation properties such as excess molar volume ($V_m^E$), excess molar isentropic compressibility ($K_{s,m}^E$), excess speed of sound ($u^E$), deviation in viscosity ($\Delta\eta$) and excess Gibbs free energy of activation for viscous flow ($\Delta G^{*E}$) were evaluated using the experimentally measured values of density ($\rho$), viscosity ($\eta$) and speed of sound ($u$). The variations in these properties with composition and temperature were used to study the interactions due to physical and chemical effects between the unlike components of the binary mixtures. Further, density values were used to estimate partial molar volumes ($\bar{V}_{m,i}$), excess partial molar volumes ($\bar{V}_{m,i}^E$) and their limiting values at infinite dilution ($\bar{V}_{m,i}^{E,\infty}$). The excess properties were fitted to Redlich-Kister polynomial equation. The correlation ability of various semi-empirical relations of viscosity was also compared using standard deviation. The excess volume data has also been rationalized by Prigogine-Flory-Patterson (PFP) theory. The calculated values of $V_m^E$ obtained from PFP theory agree with the corresponding experimental results. FT-IR spectra of these liquid mixtures have also been recorded.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Environmental sustainability and economic viability of Phase Change Materials

**PRERNA YOGESHWAR[1], JITENDRA SANGWAI[1]***

[1]Department of Chemical Engineering, Indian Institute of Technology, Madras, 600036, India
*Corresponding author: ch22d043@smail.iitm.ac.in, jitendrasangwai@iitm.ac.in

**Keywords**: Phase Change Materials, Thermal management, Life cycle analysis, Synthesis.

Phase change materials (PCMs) are gaining traction for their potential to improve energy efficiency and thermal comfort. PCMs offer significant energy savings in buildings by reducing peak cooling and heating loads. This translates to lower operational costs for heating, ventilation, and air conditioning (HVAC) systems. Studies on cold chain transportation with PCMs demonstrate reduced fuel consumption and extended product shelf life, leading to economic benefits. However, the initial cost of incorporating PCMs into building materials or transport systems can be higher compared to traditional methods. Payback periods depend on factors like energy prices, system design, and PCM material selection. PCMs contribute to environmental sustainability by reducing reliance on fossil fuels for heating and cooling. This translates to lower greenhouse gas emissions and improved air quality. The environmental impact of PCMs themselves needs consideration. Production processes of some PCMs can be energy-intensive, and some materials might raise concerns about toxicity or flammability. Bio-based PCMs offer a promising alternative with lower environmental impact. The economic viability and environmental benefits of PCMs are intertwined. Careful selection of PCMs with a focus on cost-effectiveness, energy savings, and environmentally-friendly production processes is crucial. Research and development efforts are ongoing to improve the performance and affordability of PCMs, making them a more attractive proposition for widespread adoption.

# Thermodynamic and DFT studies between 1, 2-ethylenediamine and 1, 5-Pentanediol at T = (293.15 to 313.15) K

**TANGEDA SAVITHA JYOSTNA** [1, **], **BOLLOJU SATHEESH** [2, *]

[1]Department of Chemistry, Kakatiya University, Hanamkonda-506009, Telangana, India.
[2]Department of Chemistry, Chaitanya Deemed to be University, Hyderabad-500075, Telangana, India.
*Corresponding author: e-mail: savithajyostna@gmail.com & bollucdu@gmail.com

**Keywords**: density, volumetric Properties, DFT, H-bonding

The new experimental values of density (ρ) for 1,2-ethylenediamine (EDA), 1, 5-pentanediol (PDO), and their binary mixtures were reported in the whole mole fraction of 1,2-ethylenediamine at 0.1 MPa pressure and a temperature from 293.15 K to 313.15 K. Using experimental results, molar volume ($V_m$), excess molar volume ($V_m^E$) was calculated. The observed $V_m^E$ values were interrelated to Redlich-Kister (R-K) polynomial equation. Further, utilizing Prigogine-Flory-Patterson (PFP) theory, the ($V_m^E$ was theoretically analyzed. Furthermore, apparent molar volumes ($V_{m,\emptyset,1}$ and $V_{m,\emptyset,2}$), partial molar volumes ($\bar{V}_{m,1}$ and $\bar{V}_{m,2}$), and excess partial molar volumes ($V_{m,1}^E$ and $V_{m,2}^E$) over the whole mole fraction range, also, partial molar volumes ($V_{m,1}^o$ and $V_{m,2}^o$) and excess partial molar volumes ( $V_{m,1}^{oE}$ and $V_{m,2}^{oE}$) of the 1,2-ethylenediamine and 1,5-pentanediol at infinite dilution were computed. Based on results, the hydrogen-bonding, and Lewis acid-base interactions were determined. Additionally, using density functional theory (DFT) confirmed that there were intermolecular H-bonding interactions between PDA and EDA in the binary mixtures.

## References

[1] P. Goralski, M. Wasiak, A. Bald, *J. Chem. Eng. Data* 47(1) (**2002**) 83-86.
[2] S.L. Oswal, M.M. Maisuria, *J. Mol. Liq*.100 (**2002**) 91-112.
[3] T. Singh, A. Kumar, *J. Chem. Thermodyn*. 40 (**2008**) 417-423.
[4] N.V. Sastry, S.R. Patel, *Int. J. Thermophys*. 21 (**2000**) 1153-1173.

# Analysing the molecular interactions of KCl in 0.05 mol.kg-1 aqueous 1-methyl -3 Propylimidazolium Iodide at various temperatures through physicochemical study

**VANDANA PATEL, ANKITA S. CHANDAK, SANGESH P. ZODAPE***
[1]Department of Chemistry, Visvesvaraya National Institute of Technology, Nagpur (VNIT) 440 010, Maharashtra- India.
*Corresponding author: sangesh02@gmail.com

**Keywords**: 1-methyl -3 Propylimidazolium Iodide, density, sound velocity, KCl.

In this study, we present comprehensive data on the density and speed of sound measurements for potassium chloride (KCl) within 0.05 mol.kg-1 aqueous solutions of 1-methyl-3-propylimidazolium Iodide (MPII). These measurements were conducted at temperatures of 288.15, 293.15, 298.15, 303.15, 308.15, 313.15, and 318.15 K under atmospheric pressure. The collected density data were utilized to determine the apparent molar volume of the solute at finite concentrations ( $V_{\Phi}$) and the apparent molar volume at infinitely dilute solutions ( $V_{\Phi}^{o}$) of solute. Similarly, the speed of sound data enabled the calculation of isentropic compressibility ($k_S$ ), the apparent molar isentropic compressibility of solute and limiting apparent molar isentropic compressibility of the solute at infinitely dilute solutions ($K_{S\Phi}^{o}$). Moreover, the coefficient of thermal expansion ($\alpha$), the apparent molar expansivity of the solute ( $E_{\Phi}$), and the limiting apparent molar expansivity ($E_{\Phi}^{o}$ ) were measured for ternary solutions at 293.15, 298.15, 303.15, 308.15, and 313.15 K. These thermodynamic parameters are instrumental in examining the nature of intermolecular interactions present in the studied mixtures. Our analysis includes the assessment of the solute's structure-making or structure-breaking ability in ternary solutions, using Hepler's constant. The results provide insight into the solute–solute and solute–solvent interactions, enriching our understanding of the behaviour of these mixtures in various conditions. Overall, this investigation sheds light on the complex interactions within ternary systems involving potassium chloride (KCl) and aqueous 1-methyl-3-propylimidazolium Iodide (MPII), contributing valuable data for the scientific community interested in solution chemistry and intermolecular dynamics.

## References

[1] O. Redlich, D. M. Meyer, The molal volumes of electrolytes. *Chem. Rev.* (**1964**), 64, 3.
[2] L. G. Hepler, Thermal expansion and structure in water and aqueous solution. *Can. J. Chem.* (**1969**), 47.

T1- PP 27

# Influence of methylene group and Effect of Temperature on Density, Speed of Sound, and Viscosity data of Haloarene with Linear alkanes

**MADDELA RAJI[1], S. RAVI KUMAR[2], R. KARTHIK[2], KASIBHATTA SIVA KUMAR[3], C. NAGESWARA REDDY[1*]**

[1]Thermophysical Laboratories, Department of Chemistry, Government College for Men (Autonomous), Yogi Vemana University, Kadapa -516003, Andhra Pradesh, India.
[2]Department of Physics, Saveetha School of Engineering, SIMATS University, Tamilnadu- 602105, India.
[3]Department of Chemistry, S.V. Arts College (T.T.D'S), Tirupati-517502, Andhra Pradesh, India.
*Corresponding author: e-mail: chennupallireddy@gmail.com

**Keywords**: density, speed of sound, viscosity, haloarene, FMO.

The aim of the present work is to study the influence of increase –$CH_2$ group on excess thermodynamic properties of liquid mixtures containing p-chlorotoluene (PCT) with linear alkanes ($C_7$-$C_{10}$). In this perspective, we measured density ($\rho$), speed of sound (u) and viscosity ($\eta$) for four binary liquid mixtures of PCT with n-heptane, n-octane, n-nonane and n-decane at temperature range from 298.15 to 318.15 K with interval of 5K. Further, excess volume ($V^E$), isentropic compressibility ($k_s$), excess isentropic compressibility ($k_S^E$) and excess viscosity ($\eta^E$) were calculated from experimental results and the data were fitted to the Redlich-Kister polynomial equation. Also, the correlation of measured data is performed by using PC-SAFT EoS method and by adopting the DFT/B3LYP/6–311++ G (d, p) level of theory to determine the optimized geometric structure of compounds p-chlorotoluene, n-heptane, n-octane, n-nonane and n-decane, as well as the complexes PCT + n-heptane, PCT + n-octane, PCT + n-nonane and PCT + n-decane. In order to obtain an extensive understanding of molecular interactions prevailing between component molecules were analyzed interms of geometric and electronic features of the above-mentioned complex compounds, Frontier Molecular Orbitals (FMO) analysis and quantum chemical descriptors, such as ionization potential, electron affinity, global hardness, and orbital energy gap, have been performed.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Exploring the Solvation Behavior of D-Glucose in Aqueous Imidazolium-based Ionic Liquid Solution at different Temperatures

**ANKITA S. CHANDAK, SANGESH P. ZODAPE***

Department of Chemistry, Visvesvaraya National Institute of Technology (VNIT), Nagpur- 440 010, Maharashtra, India

*Corresponding author: e-mail: szodape@chm.vnit.ac.in, sangesh02@gmail.com

**Keywords:** Density; Sound velocity; Ionic liquid; D-Glucose; Limiting apparent molar volume; Limiting apparent molar isentropic compressibility.

The interactions between biopolymers, specifically polysaccharides, and ionic liquids (ILs) are pivotal for elucidating solvation behavior and molecular-level mechanisms governing biopolymer dissolution and functionalization processes. Accurate reference data on the physicochemical properties of systems comprising imidazolium-based ILs and biopolymer model compounds, such as glucose in aqueous solution, are essential for gaining comprehensive insight into structural interactions. In this regard, we measured volumetric and compressibility studies of D-glucose in 0.05, 0.10, and 0.15 mol. kg$^{-1}$ aqueous 1-methylimidazole trifluoromethanesulfonate [MIm][OTf] ionic liquid solutions across concentration ranges (0.06 to 0.15 mol.kg$^{-1}$) at different temperatures (288.15-318.15 K), respectively. To understand the strength and extent of solute-solvent interactions, several thermophysical parameters, including the apparent molar volume of solute, isentropic compressibility of solution and apparent molar isentropic compressibility of solute, were derived from estimated experimental density and sound velocity data. Additionally, transfer parameters of D-glucose from aqueous to aqueous [MIm][OTf] solutions were determined. The results reveal significant interactions between ions of [MIm][OTf] and hydrophilic groups of D-glucose. This study discusses the complex interplay between [MIm][OTf] ionic liquid and D-glucose molecules, advancing our understanding of cellulose chemistry and holding significant implications in materials science, biotechnology, and environmental applications.

## References

1. A.S. Chandak, A. Jain, S.P. Zodape, J. Mol. Liq. 383 (2023) 122100.
2. V.Singh, P.K. Chhotaray, Nasarul Islam, R.L. Gardas, J. Chem. Thermodyn. 103 (2016)7–1.
3. A. Jain, S.P. Zodape, J. Mol. Liq.363 (2022) 119817.
4. H.L. Friedman, C.V. Krishnan, J Solution Chem. 2 (1973) 119–140

**T1- PP 29**

# Thermal properties of modified chitosan-based sponges with enhanced haemostatic properties for wound healing applications

**Rizos-Evangelos Bikiaris**[1,2], **Ioanna Koumentakou**[1,2], **Despoina Meimaroglou**[1], **George Z. Kyzas**[2]
[1] Laboratory of Polymer and Colors Chemistry and Technology, Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece
[2] Hephaestus Laboratory, Department of Chemistry, School of Sciences, Democritus University of Thrace, Kavala 65404, Greece
*Corresponding author: e-mail: rizosbikiaris@gmail.com

**Keywords**: chitosan modification, haemostasis, wound healing, TGA

The initial phase of wound healing, haemostasis, is activated upon injury and serves to control bleeding, while forming a protective barrier. In cases of severe wounds, where this process is impaired, the use of haemostatic agents becomes necessary. Despite recent advancements in their development, many of these agents are inefficient in halting severe bleeding, expensive, or carry risks such as unintended blood clotting. Chitosan was selected due to its biological properties, including biocompatibility, non-toxicity, antibacterial activity, and haemostatic properties. It is extensively employed in wound healing applications. However, CS solubility is restricted to acidic conditions, limiting its usability. Generally, chemical modifications enhance chitosan's processability, solubility, antimicrobial efficacy, and its capacity to interact with other substances.

In the present work, a grafted chitosan derivative was prepared through free-radical polymerization, using 2-acrylamido-2-methyl-1-propanesulfonic acid (AAMPS) comonomer to further improve the inherent haemostatic and antimicrobial properties. Porous sponges of CS-g-AAMPS were then fabricated *via* a modified thermal-induced phase separation process. The structural properties of the prepared sponges were evaluated using FT-IR spectroscopy, their crystallinity was examined via XRD (Fig 1a), and finally, TGA analysis was performed in order to examine the effect of modification on thermal stability (Fig 1b).

(a)

(b)

Figure 1: (a) XRD spectra of CS, AAMPS monomer and CS-AAMPS derivative, (b) TGA thermograms of neat CS and the prepared CS-AAMPS.

**Acknowledgments:** The authors wish to acknowledge co-funding of this research by European Union-European Regional Development Fund and Greek Ministry of Education, Research and Religions/EYDE-ETAK through program EPANEK 2014-2020/Action “EREVNO-DIMIOURGO-KAINOTOMO” (project T2EΔK-00275).

# Exploration of interactions between L - Aspartic acid and Saccharides in aqueous medium at T= (293.15-313.15) K: Physicochemical and Spectroscopic approach

**RUPESH KUMAR PRADHAN, SULOCHANA SINGH ***

Department of Chemistry, ITER, Siksha O Anusandhan Deemed to be University, Odisha

*Corresponding authors' email id: ssingh14dec2015@gmail.com

**Keywords:** Apparent molar volume; Hepler's constant; transfer parameters; taste behaviour; UV spectral analysis.

In this study, we report the density, viscosity, taste behavior and UV- Vis spectrophotometry results of L-Aspartic acid (Asp) in aqueous solutions of L-arabinose and D-xylose over an integral composition regime (2.0 wt%, 2.5 wt%, and 3.0 wt%) at atmospheric pressure (P = 101 kPa) and at temperature ranges of (293.15, 298.15, 303.15, 308.15, and 313.15) K. The various densimetric and rheological parameters such as apparent molar volume ($V_{\phi}$), apparent molar volume at infinite dilution ($V_{\phi}{}^{0}$), apparent molar isobaric expansion at infinite dilution ($E\phi^{0}$), Hepler's constant ($\partial^{2}V\Phi^{0}\ \partial T^{2}\!/$) P , relative viscosity (ηr ), viscosity coefficients (BJ and AF ), Gibbs free energy of activation of viscous flow of solvent and solute (Δμ1 #,0 and Δμ2 #,0 respectively), and corresponding change in enthalpy ΔH2 #,0 , entropy $\Delta S_2$ #,0 , apparent molar volume of transfer at infinite dilution ($V_{\phi}$,$tr^{0}$ ) viscosity B-coefficients of transfer (BJ,tr), interaction coefficients (using the McMillan-Mayer theory), dB/dT and solvation number (Sn) have been calculated using the experimentally collected physical characteristic data (density and viscosity). Variation of these parameters with concentration and temperature were analyzed in the light of ion-ion, ion-dipole and ion-hydrophilic interactions between solute (L-Aspartic acid)-cosolute (L-arabinose and D-xylose) in aqueous medium. An effort has also been made to compare the taste behaviours of the amino acid in water and in an aqueous solution of saccharides, as the taste behaviour is separated into four basic taste qualities in distinct ranges. To access different common intermolecular interactions in the systems under consideration, the cosphere overlap model has also been used. A detailed evaluation of the results from the thermodynamic and physicochemical parameters shows that Asp acts as a structure builder when L-arabinose/D-xylose is present. The preservation of effective ionic interactions in the studied systems was further confirmed by UV spectral analysis.

**References**

[1] P.K. Banipal, A.K. Hundal, Viscometric studies on saccharides in aqueous magnesium chloride solutions at T=(288.15 to 318.15)K, J. Chem. Thermodyn. 51 (2012) 70–76. https://doi.org/10.1016/j.jct.2012.02.016.

[2] A.K. Nain, M. Lather, Study of solute–solute and solute–solvent interactions of l -serine in d - xylose/ l- arabinose + water solutions using volumetric, ultrasonic and viscometric methods at different temperatures, Phys. Chem. Liq. 53 (2015) 599–618

[3] KK Athira, RL Gardas, Interactions of ammonium based ionic liquids with DNA in aqueous medium through Volumetric, acoustic and viscometric properties, J. Mol. Liq, 389 (2023) https://doi.org/10.1016/j.molliq.2023.12285

**T1- PP 31**

# Kinetic And Thermodynamic Parameters Of Reactions In Reverse Micelles

**K.V.NAGALAKSHMI[1], P.SHYAMALA[2*], B.LEELA KUMARI[3]**

1Department of chemistry, Gayatri Vidya Parishad College of Engineering (A),
Visakhapatnam530048, Andhra Pradesh, India.
*2Department of Chemistry, Andhra University, Visakhapatnam - 530003, Andhra Pradesh,
India.

3Department of Chemistry, St. Joseph college , Visakhapatnam - 530003, Andhra Pradesh,
India.

*Corresponding Author: shyamalapulipaka06@gmail.com

Reverse micellar systems are known to exhibit catalytic effects which result from concentration of reactants in the nano water pool and the it's anomalous physicochemical properties. In this work, we have studied the catalytic effect of reverse micelles on a number of reactions. The study investigates the kinetics and thermodynamic properties of three reactions carried in both aqueous and CTAB reverse micellar media. The dissociation of $\{Fe(tptz)_2\}^{2+}$ is notably slow in water but accelerates significantly in CTAB micelles. In another reaction, the reaction between toluidine blue and periodate is forty times faster in CTAB micelles compared to water, whereas the organic reaction involving paranitrophenyl acetate and hydrazine is twenty times slower in CTAB micelles. The difference in rates between reverse micellar systems and aqueous medium for all the three reactions are explained in terms of thermodynamic parameters. The activation parameters were determined by carrying out the reactions at different temperatures. Good linear plots according to Arrhenius equation ($\log k' = \log A - Ea/2.303RT$) were obtained. Activation parameters $\Delta H^{\neq}$ and $\Delta S^{\neq}$ were determined according to Eyring equation $k' = (kBT/h) \exp(-\Delta H^{\neq}/RT) \exp(\Delta S^{\neq}/RT)$ for all the reactions mentioned. Activation energy analysis using the Eyring equation reveals that reactions catalysed by CTAB micelles exhibit lower activation energies compared to aqueous environments, whereas reactions hindered by micellar surroundings display higher activation energies.

18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024

# Thermodynamic Studies of Ionic Interactions in Aqueous Solutions of Diethylammonium based Protic Ionic Liquids

**<u>GURUPRASAD J. HASOLKAR</u>[1], PRATIKSHA P. GAVHANE[1] AND DILIP H. DAGADE[1]***

*1Department of Chemistry, Shivaji University, Kolhapur – 416 004*
*Corresponding author: e-mail: dhd_chem@unishivaji.ac.in

**Keywords-** Partial molar volume, Compressibility, hydration number, Osmotic and activity coefficient

The ammonium based protic ionic liquids (PILs) have applications in the pharmaceutical industries for the solubility and stability of the active pharmaceutical ingredients (APIs) and its better utility can only be achieved if physicochemical and molecular level understanding of ion-ion and ion-solvent interactions is available. Seen in this light, the density measurements in the temperature range of 298.15 K to 313.15 K and speed of sound measurements at 298.15 K were made for the aqueous solutions of the diethylammonium based glycolate (DEAG) and lactate (DEAL) PILs in the concentration range of ~0.02 $mol\cdot kg^{-1}$ to ~1.00 $mol\cdot kg^{-1}$ from which apparent and partial molar volumes, coefficient of thermal expansion, compressibility, internal pressure and concentration dependent hydration numbers were obtained. Also, osmotic coefficient for the aqueous solutions of DEAG and DEAL at 298.15 K in the concentration scale of ~0.01 $mol\cdot kg^{-1}$ to ~1.00 $mol\cdot kg^{-1}$ were determined using vapor pressure osmometer and used to obtain water activities and mean molal activity coefficients for PILs in aqueous medium. The McMillanMayer theory of solutions was applied to account the nonelectrolyte contribution in the aqueous solutions of the PILs. Additionally, the osmotic second virial coefficient obtained from it gives information on oppositely charged ion-pair – ion-pair (electrically neutral ion-pairs) interactions for PILs in the aqueous medium. The application of Pitzer model for 1:1 electrolyte solution yielded the Pitzer ion interaction parameters $\beta^0$ and $\beta^1$ for which experimental osmotic coefficient data were fitted using Pitzer equations through least square fit method. The $\beta^1$ value for DEAG signify the like ions (cation-cation or anion-anion) interactions are favorable whereas the negative $\beta^1$ values for DEAL indicates the oppositely charged ion pairs formation. The results obtained were further discussed in terms of ion-ion, ionsolvent interactions, cooperative hydrogen bonding, etc.

## References-

(1) Dagade, D. H.; Madkar, K. R.; Shinde, S. P.; Barge, S. S. *J. Phys. Chem. B, 117* (4), (**2013**) 1031–1043.
(2) Gardas, R. L.; Dagade, D. H.; Coutinho, J. A. P.; Patil, K. J. *J. Phys. Chem. B, 112* (11) (**2008**) 3380–3389.

18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024

# Observation of the α-β phase transition of Quartz by differential scanning calorimeter

**Haruka Abe**[1]*

[1]National Metrology Institute of Japan (NMIJ), National Institute of Advanced Industrial Science and
Technology (AIST), Tsukuba, Ibaraki 3058563, Japan
*Corresponding author: e-mail: abe-haruka@aist.go.jp

**Keywords**: Phase-transition, DSC, $SiO_2$,

The α-β phase transition of quartz, $SiO_2$, which Le Chatelier discovered in 1889 [1], is known to occur near 850 K. Since the existence of an incommensurate phase in the α-β phase transition was found in the early 1980s, various studies about this phenomenon have been carried out [3-6]. However, it is hard to say that we fully understand it.

One of the thermal approaches to observe this phenomenon is the measurement by a differential scanning calorimetry. Dolino et al. tried to observe the behavior of an intermediate phase in the α-β phase transition using a differential scanning calorimeter [2]. In conclusion, they found the existence of an intermediate, or incommensurate, phase on a temperature range of 1.3 K between β and α phase upon cooling. However, the existence of the incommensurate phase was not found during the heating process.

In the presentation, the precise observation of the α-β phase transition phenomena and the measurement technique by the differential scanning calorimeter are reported in detail.

## Reference

[1] H. Le Chatelier, C. R. Acad. Sci. (Paris), 108 (1889) 1046.
[2] G. Dolino, J. P. Bachheimer, C. M. E. Zeyen, Solid State Commun. 45 (1983) 295.
[3] I. Hatta, A. J. Ikushima, Jpn. J. Appl. Phys. 20 (1981) 1995.
[4] M. Matsuura, H. Yao, K. Gouhara, I. Hatta, and N. Kato, J. Phys. Soc. Japan, 54 (1985) 625.
[5] H. Yao, I. Hatta, Thermochimica Acta, 266 (1995) 301.
[6] N. Kato, K. Gouhara, J. Appl. Phys. 24 (1985) 157.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Alternative Solvents for Efficient $CO_2$ Capture: The Role of Basicity, Free Volume, and their Thermodynamic Properties

**INDRAJIT DAS[1], RAMESH L. GARDAS[1*]**

[1]Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036, India
*Corresponding author: e-mail: gardas@iitm.ac.in

**Keywords: Ionic liquids, $CO_2$ capture, thermodynamic property, Basicity**

Conventional absorbents/solvents face several challenges, prompting the search for alternative solvents for efficient $CO_2$ capture. In this context, room-temperature ionic liquids (ILs) have shown superior performance for $CO_2$ capture and are identified as potential absorbents [1]. These alternative solvents offer distinct advantages, such as reduced volatilization and improved regeneration [2]. Designing new functionalized ILs for $CO_2$ capture requires careful consideration of the thermodynamic properties of IL-$CO_2$ systems. Among the various types of ionic liquids, protic ionic liquids (PILs) are particularly promising due to their straightforward synthesis processes and unique characteristics. This study focuses on developing polyamine-based PILs for efficient and selective $CO_2$ capture from exhaust gases.

We extensively examined the basicity (pKa) and free volume of ILs, as these are crucial parameters for higher $CO_2$ absorption. Additionally, we investigated the effects of temperature, pressure, and the alkyl chain length of anions on $CO_2$ absorption. Based on these findings, the "deactivated IL" model [3] was employed to derive the chemical equilibrium constants of $CO_2$ with the ILs at various temperatures. From the equilibrium constant data, we calculated other thermodynamic properties of absorption, such as reaction Gibbs energy, reaction enthalpy, and reaction entropy.

Furthermore, $^{1}H$ NMR, $^{13}C$ NMR, and FT-IR spectroscopy were used to study the interactions between $CO_2$ and the ILs, confirming the formation of carbamate peaks indicative of chemical absorption. We correlated the $CO_2$ absorption capacities of ILs with experimental parameters like free volume and thermodynamic properties, including enthalpy and Gibbs free energy. The viscosity of ILs was measured both before and after $CO_2$ absorption, and regeneration energy was also calculated. Finally, we investigated the $CO_2$ absorption-desorption cycles of the ILs, as the recycling performance of ILs is crucial for industrial use in $CO_2$ capture.

**References**

[1] Das, I., Swami, K.R. and Gardas, R.L., Influence of alkyl substituent on thermophysical properties and $CO_2$ absorption studies of diethylenetriamine-based ionic liquids, *Journal of Molecular Liquids*, *371*, (**2023**) 121114.

[2] Blanchard, L.A., Hancu, D., Beckman, E.J. and Brennecke, J.F., Green processing using ionic liquids and $CO_2$. *Nature*, 399, (**1999**) 28-29.

[3] Huang, Y., Cui, G., Wang, H., Li, Z. and Wang, J., Absorption and thermodynamic properties of $CO_2$ by amido-containing anion-functionalized ionic liquids, *RSC advances*, *9*, (**2019**) 1882-1888.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Exploration of volumetric, optical, thermodynamic, FT-IR and DFT studies of binary mixtures of ethanoic acid with higher 1-alkanols at different temperatures

**P. ANNAPURNA[1], SREENIVASULU KARLAPUDI[2], KASIBHATTA SIVA KUMAR[3], B. MAHESH[1*]**

[1]Thermophysical Laboratories, Department of Chemistry, Government College for Men (Autonomous), Yogi Vemana University, Kadapa -516003, Andhra Pradesh, India.
[2]Department of Chemistry, Sree Rama Engineering College, Tirupati-517507, Andhra Pradesh, India.
[3]Department of Chemistry, S.V. Arts college (T.T.D'S), Tirupati-517502, Andhra Pradesh, India.
*Corresponding author: e-mail: mahi.babu3@gmail.com

**Keywords**: Density, Excess volume, 1-alkanol, FT-IR, Density Functional Theory.

To understand the nature and type of molecular interactions between ethanoic acid and 1-alkanols ($C_8$-$C_{10}$), measurements such as density (ρ), speed of sound (u) and refractive index ($n_D$) at T = (298.15 K - 323.15) K and 0.1 MPa have been carried out. Excess volume ($V^E$), isentropic compressibility ($k_s$), excess isentropic compressibility ($k_s^E$), excess refractive index ($n_D^E$) was calculated from experimental results and fitted to the Redlich-Kister polynomial equation. As well as, the variation of these excess thermodynamic properties with composition and temperature is discussed in terms of molecular interaction between component molecules in liquid mixtures and their interacting abilities are compared. Further, FT-IR spectra of pure liquids and their mixtures at various concentrations were recorded and Density Functional Theory (DFT) calculations for 3 sets of binary systems was carried out for all binary systems in order to know the strength of molecular interactions that are existing between component molecules in liquid mixtures.

# Physicochemical Properties of Biogenic Monoamine Neurotransmitters: Volumetric, Viscometric and Thermoacoustic Investigations

**PRANALI Y. UMREDKAR[1*], SNEHA T. BANKAR[1], VIJAY M. TANGDE[1], NIRAJ T. KHATY[2], SUDHAKAR S. DHONDGE[3]**

[1]Department of Chemistry, Rashtrasant Tukadoji Maharaj Nagpur University, Nagpur, 440033, India

[2]Department of Chemistry, Laxminarayan Innovation Technological University, Nagpur,440033, India.

[3]P.G. Department of Chemistry, S. K. Porwal College Kamptee, Dist. Nagpur, 441001, India

*Corresponding author: Pranali Y. Umredkar e-mail: pranali1u@gmail.com

**Keywords**: Biogenic amine, compressibility, density, viscosity, speed of sound

Phenylethylamine and its derivatives, including Tyramine and Dopamine, are natural neuromodulatory trace amines formed by enzymatic decarboxylation of amino acids. As monoamine alkaloids, they act as stimulants in the human brain, playing various indispensable biological roles, also showcasing the potential as anti-proliferative agent and cancer cell markers. In context of understanding the precise biochemical mechanisms underlying their actions, the present study undertakes the experimental determination of density, speed of sound and viscosity data over the concentration range of 0.02-0.2 mol kg$^{-1}$ and temperature ranging from 288.15 K to 318.15 K, covering the span of human body temperature. Various thermodynamic parameters were scrutinized shedding light on their physiochemical behavior in the aqueous environment. The limiting apparent molar volume of solute ($V_\phi^0$) & the corresponding $S_v$ values substantiate dominant amine-water interactions wherein significant hydrophobic hydration was marked by the highly negative compressibility ($K_{s,\emptyset}^0$) values. In the same vein, the identification of Hepler's constant ($\partial^2 V_\phi^0/\partial T^2$), $B-$ coefficient and , $dB/dT$ value underscores chaotropic trait of the studied molecules. Moreover, the strong positive $\Delta\mu_2^{0\#}$ values manifest easily accessible ground state over transition state, while the negative $\Delta S_2^{0\#}$ and positive $\Delta H_2^{0\#}$ signifies strong hydrogen bonding and orderedness associated with the activated state. The study thus reveals the profound interactions, providing further insights into molecular aspects and the binding forces involved

# Thermodynamics of Thermal Degradation of Poly(Ethylene 2,5-Furan Dicarboxylate) Nanocomposites for Food Packaging applications

**JOHAN STANLEY[1], DIMITRA A. LAMBROPOULOU [1,2*], DIMITRIOS N. BIKIARIS[1]**
[1]Dpartment of Chemistry, Aristotle University of Thessaloniki, GR–541 24 Thessaloniki, Greece
[3]Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Balkan Center,
GR-570 01 Thessaloniki, Greece
*Correspondence: dlambro@chem.auth.gr

**Keywords**: Poly(ethylene 2,5-furan dicarboxylate), Nanoparticles, Nanocomposites, Thermal properties, Decomposition mechanism

Nanoparticles with at least one dimension of a few nanometres are incorporated into a biobased polymeric matrix to create innovative materials for food packaging applications. [1] In present work, Poly(ethylene 2,5-furan dicarboxylate) (PEF) based nanocomposites containing different nanoparticles like Ag, $TiO_2$, ZnO, $ZrO_2$ Ce-Bioglass, have been synthesized via in-situ polymerization techniques targeting food packaging applications.

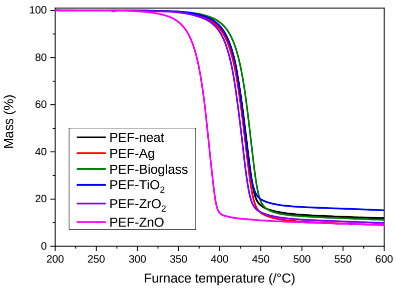


Fig. 1: TGA thermograms of neat PEF and PEF nanocomposites at a heating rate of 20 °C/min under a nitrogen atmosphere

Thermogravimetric analysis results proved that, except PEF-ZnO nanocomposite, all the other nanocomposites exhibited good thermal stability without serious mass loss until 330°C as displayed in Fig. 1. The degradation process of PEF is influenced by ZnO nanoparticles, as demonstrated by the results of thermal decomposition kinetic study. On the other hand, Ce-Bioglass nanoparticles slow down the degradation process and prevent volatile chemicals from diffusing, which increases the PEF-Bioglass nanocomposite's thermal stability. [2] Overall, the findings demonstrate that all of the other nanocomposites aside from the PEF-ZnO nanocomposite had noteworthy thermal characteristics appropriate for thermomechanical recycling or the processing of packaging material.

## Acknowledgments

This work was supported by the project “Advanced research and Training Network in Food quality, safety and security” FoodTraNet - H2020-MSCA-ITN-2020 GRANT AGREEMENT, No 956265

## References

[1] N.A. Al-Tayyar, A.M. Youssef, R. Al-hindi, , *Food Chem*, 310 **(2020)** 125915.
[2] K. Chen, C.A. Wilkie, S. Vyazovkin, *J. Phys. Chem. B*, 111 **(2007)** 12685

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Ionic liquids as a dual solvocatalyst for esterification reactions

**GEETHANJALI M, SUNITA RAJAMANI***

Department of Chemistry, School of Chemical Sciences, St. Joseph's University, Langford Road,
Bengaluru 560027
*Corresponding author email: sunita.rajamani@sju.edu.in

**Keywords:** nitrogen based ILs, Hammet acidity, thermal stability, esterification

Esterification is a fundamental chemical process with wide industrial applications, particularly in the production of esters for use in flavors, fragrances, and solvents. The esterification reactions of some alcohols were targeted using acetic acid. In this study, we explore the use of nitrogen-based ILs as a sustainable alternative to traditional solvents for this reaction. The primary objective is to assess the efficiency and environmental benefits of conducting the esterification in ionic liquids, a class of solvents known for their low volatility and recyclability. The reaction efficiency, yield, and Hammet acidity were systematically evaluated. Our findings indicate that ILs not only enhance the reaction rate and yield but also offer significant environmental advantages by reducing volatile organic compound emissions and enabling solvent recovery and reuse. The results demonstrate that employing ILs in esterification processes aligns with the principles of green chemistry, offering a viable path towards more sustainable industrial practices. This study focuses on the potential of ILs to replace traditional solvents, thereby minimizing the environmental footprint of chemical manufacturing.

### References

1. J. Fraga-Dubreuil, K. Bourahla, M. Rahmouni, J. Pierre Bazureau, J. Hamelin, Catalysis Communications, 3 (2002), 185.
2. L. Mullins and J.A. Sullivan, Sustain. Chem. 1 (2020), 138

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Stability of Current Collectors in Ionic Liquid Electrolytes for Aluminum-Ion Batteries

**SOMENATH PANDA, VIKAS SHARMA, RAMSAGAR VOORADI, VENKATA SURESH PATNAIKUNI, MANOHAR KAKUNURI***

Center of excellence on batteries, National Institute of Technology Warangal, Warangal-506004, India

Corresponding author: e-mail: manohar@nitw.ac.in

**Keywords**: Al-ion battery, Current collector, Deep eutectic solvents, Electrolytes

Aluminium ion batteries (AIB) are emerging as a potential low-cost energy storage solution considering the abundance of materials, non-flammability and adequate energy density among others [1]. However, the high cost of the non-aqueous ionic liquid-based electrolytes and their corrosive effect on the current collectors and cell-casings need to be tactically addressed for AIBs to make them commercially feasible [2]. In this study, two cost-effective ionic liquid analogues, AlCl3-Urea and AlCl3-Acetamide, were used as electrolytes to investigate the corrosion behavior of four metallic current collectors: stainless steel, copper, nickel, and molybdenum (Mo) in a full-cell configuration. A comprehensive analysis was conducted using electrochemical characterization techniques, including Electrochemical Impedance Spectroscopy (EIS), Cyclic Voltammetry (CV), and Galvanic Charge-Discharge (GCD), to assess the stability of each current collector in the electrolytes. Additionally, ongoing morphological studies aim to elucidate the precise nature of corrosion in these electrolytes. This study will help identify the optimal electrolyte-current collector combination to enhance the performance and stability of AIBs.

**References**

[1] MC Lin. *et al.* An ultrafast rechargeable aluminium-ion battery. *Nature* 520 (**2015**), 324–328

[2] P. Meng *et al*. Electrolyte design for rechargeable aluminum-ion batteries: Recent advances and challenges. *Energy Storage Materials* 63 (**2023**) 102953

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Redox Active Deep Eutectic Solvents (DES) for Energy Storage

**KONDEPOGU DEVAIAH, RAMESH L GARDAS***

Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036, India
*Corresponding author: e-mail: gardas@iitm.ac.in

**Keywords**: DES, Energy storage, Redox activity, Electrolyte

## Abstract

Deep Eutectic Solvents are emerging as an alternative electrolyte in energy storage which Ionic Liquids (ILs) possess physical properties like, less toxic, low vapor pressure, corrosion resistant, high ionic conductivity, surface tension and eco-friendly and bio-degradable it has similar properties like Ionic Liquids (ILs). Where as Ionic liquids are expensive, forms corrosion at the aluminum current collector side also these materials have lesser mobility due to their viscosity to overcome this challenge researchers are focusing on Deep Eutectic Solvents (DES). These Materials will not form any type of corrosion at the current collector interfaces basically synthesis of DES materials requires lesser cost when compared with synthesis of redox active ILs. So, the need of this redox active materials mainly for electron transfer in between the Electrode Electrolyte Interface (EEI) [1]. This DES materials have at least one hydrogen bond acceptor (HBA) choline chloride, metal halides and quaternary ammonium analogues and should have one hydrogen bond donor (HBD) such as amide, alcohol and carboxylic acid molecules. Some of the DES moiety's like reline, ethaline and glycerine are not redox active so these type mixtures are used for non-aqueous media for synthesis. If the components have one metal halide or redox active moiety (Eutectic system) occurs to electrode deposition, stripping and organic redox reactions [2].

### References

[1] R. Puttaswamy, C. Mondal, D. Mondal, D. Ghosh, Sustainable Materials and Technologies 33 (2022) e00477.

[2] C. Zhang, L. Zhang, G. Yu, Accounts of Chemical Research 53 (2020) 1648–1659.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Investigating the Effect of Nd+3 Substitution on the Supercapacitor Performance of Cobalt Copper Ferrites

**V. M. GHARE*, R. N. SHIRSAT, A. V. SALKER**

School of Chemical Sciences, Faculty block E, Goa University, Taleigao plateau, Goa, India 403206
*Corresponding author: e-mail: vipulghare@gmail.com

Metal ferrites have outstanding electrochemical characteristics owing to the numerous oxidation states of the metal ions, making them promising materials for addressing both sustainable energy conversion and storage and growing environmental issues.1 Therefore, nanocrystalline transition metal ferrites such as Cu0.5Co0.5Fe2O4 and Cu0.5Co0.5Fe2- xNdxO4 (x= 0.01, 0.02, 0.03, 0.04, and 0.05) were synthesized using combustion method and were used as electrode materials for supercapacitor applications. Our work investigates the effect of Nd+3 substitution on the structural, morphological and electrochemical performance of the synthesized compounds. The synthesized materials were characterized using XRD, IR, FESEM, Raman, and BET studies. The findings illustrated the formation of a single-phase spinel ferrite as proved from XRD data. Additionally, it was also observed that Nd+3 substitution directly influenced the lattice parameters and the average crystallite size of substituted ferrites and the electrochemical performance, thus proving that the said compound act as supercapacitor material.

**References**

[1] Al Kiey, S. A.; Ramadan, R.; El-Masry, *Appl. Phys. A Mater. Sci. Process*, 128(6) (**2022**) 1–13.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Full solar spectrum active Fe-doped CuSe nanostructure for enhanced photocatalytic activity: Structural, optical and photocatalytic performance investigation

**VIKAS KUMAR, AWNISH KUMAR TRIPATHI***

Department of Physics, National Institute of Technology Kurukshetra, Kurukshetra 136119, India
*Corresponding author email: awnish1982@nitkkr.ac.in

**Keywords:** CuSe photocatalyst, Fe-doped CuSe nanostructure, Solar spectrum active photocatalyst, Photocatalytic efficiency, Multiple dye degradation

Developing a full solar spectrum active photocatalyst with enhanced photocatalytic activity has been challenging but crucial for achieving a sustainable environment. We report an in-depth experimental investigation on the photocatalytic performance of Fe doped CuSe nanostructures and exploration for an optimal Fe doping concentration for achieving improved full solar spectrum activity. XRD analysis shows that Fe doping changes the CuSe crystal phase from hexagonal to cubic beyond a certain doping concentration, suggesting a solubility limit of Fe in CuSe lattice. FESEM and HRTEM analyses reveal that the prepared CuSe has a nanoplate morphology, and becomes agglomerated with Fe doping. The EDS and XPS analyses are used to investigate the purity and stoichiometry of synthesized Fe-doped CuSe samples. The conventional optical characterizations show a slight red shift in the absorption edge and a notable suppression in photoluminescence intensity for Fe doped CuSe compared to the undoped CuSe samples. Herein, improved degradation rate for Fe-doped CuSe is observed compared to undoped CuSe for the model dye Methylene Blue. The wastewater treatment performance, of prepared doped samples, is also investigated for various industrial dyes namely Methylene Orange, Malachite Green, Naphthol violet and Congo red. The improved degradation efficiency strongly implies that Fe doping offers substantial promises for advancing in the utilization of CuSe and its variants in photocatalytic wastewater treatment. Through our analysis and detailed discussion, we are optimistic that our findings would provide insights to the researchers interested in achieving a full solar spectrum active photocatalyst and would support the industries who are facing challenges due to wastewater management issues.

**References**

[1] C. Chen, J. Zhang, X. Xiong, J. Lin, S. Yang, J. Xi, Z. Kong, , *International Journal of Hydrogen Energy,* 47 (**2022**) 28879–28893.
[2] X. Wang, Z. Miao, Y. Ma, H. Chen, H. Qian, Z. Zha, *Nanoscale,* 9 (**2017**) 14512–14519.
[3] M. Nouri, R. Yousefi, N. Zare-Dehnavi, F. Jamali-Sheini, *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 586 (**2020**).

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

---

# Adsorption of D-A'-π-A Carbazole dyes on $TiO_2$ surface for Dye-Sensitized Solar Cell Applications

**VIPIN KUMAR AND PRABHAKAR CHETTI***

Department of Chemistry, National Institute of Technology (NIT), Kurukshetra-136119, India.
*Email: chetty_prabhakar@yahoo.com

**Keywords**: DSSCs, Photovoltaics, DFT/TD-DFT, Carbazole dye.

## Abstract:

In this work, we investigated adsorption of D-A'-π-A dyes on $(TiO_2)_{16}$ surface and investigated the effects of different π-bridges on the optical and photovoltaic characteristics for Dye-Sensitized Solar Cells (DSSCs). We have shown that the light sensitivity of dyes may be adjusted from visible to near-infrared wavelengths by varying the π-spacer unit. The performance of the D-A'-π-A system has been evaluated in terms of various photovoltaic parameters such as the light harvesting efficiency (LHE), highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO) HOMO-LUMO energy gap ($\Delta E_g$), excited-state oxidation potential ($E^{dye*}$), total reorganization energy ($\lambda_{total}$). The short circuit current density ($J_{SC}$), free energy of electron injection ($G_{inject}$), open-circuit voltage ($V_{OC}$), and power conversion efficiency are also calculated by using DFT/TD-DFT methodology. This study sheds light on the existing and potential future trends in DSSCs for improved solar device performance and enhanced solar light harvesting.

**References**

[1]. V. Kumar, P. Chetti, J. Mol. Graph. Model. 123 (2023) 108512.
[2] A. Tripathi, A. Ganjoo, P. Chetti, Solar Energy 209 (2020) 194.
[3]. S. Koudjina, V. Kumar, G. Y.S. Atohoun, J. D. Gbenou, P. Chetti, J. of Photochem. And Photobio., A: Chemistry 442 (2023) 114772.
[4] V. Kumar, P. Chetti, J. Comput. Biophys. Chem. 22 (2023) 983.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Comparative study of photocatalytic degradation of dye using $Fe_3O_4$ using electromagnetic radiations of various energies

**PRAFUL W. JAMBHULE[1]*, INDRANI B. DAS SARMA[1,2], NIRAJ T. KHATY[3], VIJAY M. TANGDE[1]**

[1]Department of Chemistry, Rashtrasant Tukadoji Maharaj Nagpur University, Nagpur 440 033, India
[2]Department of Chemistry, Jhulelal Institute of Technology, Koradi Road, Lonara , Nagpur 441 111, India
[3]Department of Chemistry, Laxminarayan Innovation Technological University, Nagpur – 440 033, India
*Corresponding author: e-mail: prafuljambhul97@gmail.com

**Keywords:** DES, Fe3O4, photocatalyst

The environmental impact due to untreated textile waste water consisting of various organic dyes and pigments are well-known. The tertiary treatment of the same involves adsorption techniques on various types of adsorbents. This increases the pollution load as after a few cycles of adsorption and desorption the material renders ineffective. Hence, the more efficient way of reducing the organic wastes is mineralizing the waste to basic non-toxic molecules which has lesser environmental impact. Hence photocatalysis of the waste would be a better alternative [1]. In the present work, nanoscale magnetite ($Fe_3O_4$) synthesized by co-precipitation method in the Deep Eutectic Solvent (DES) which is used as photocatalyst [2]. The $Fe_3O_4$ was characterized by established methods which revealed that it has an inverse spinel structure. The nano-magnetite was used as a photocatalyst to study degradation of Crystal Violet in aqueous medium. The study was carried out in ultraviolet, visible and gamma radiations. The synergistic effect of $H_2O_2$, $H_2O_2$ + $TiO_2$, $Fe_3O_4$ and $Fe_3O_4$ + $H_2O_2$ on dye degradation and its kinetics were studied. It was found that the efficiency of $Fe_3O_4$ emerge out higher in catalyzing the degradation of the dye.

## References

[1] A. B. Mapossa, W. Mhike, J. L. Adalima, and S. Tichapondwa, 'Removal of organic dyes from water and wastewater using magnetic ferrite based titanium oxide and zinc oxide nanocomposites: A review', Catalysts, vol. 11, no. 12. MDPI, Dec. 01, 2021.

[2] F. Chen, S. Xie, J. Zhang, and R. Liu, 'Synthesis of spherical Fe3O4 magnetic nanoparticles by coprecipitation in choline chloride/urea deep eutectic solvent', Mater Lett, pp 177–179, 2013

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# A Computational Study on Transition metal doped MOF-5 for Carbon Capture

**DIKSHA PRAVEEN PATHAK[1]*, JITENDRA SANGWAI[1]**

[1]Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai-600036, India
*Corresponding author: e-mail: ch23d406@smail.iitm.ac.in

**Keywords:** Climate change, Carbon Capture, Density functional Theory, Metal Organic Frameworks.

The escalating levels of carbon dioxide ($CO_2$) in the atmosphere, primarily driven by human activities such as industrial processes and fossil fuel combustion, pose a critical threat to global climate.[1] It is crucial to create affordable materials that are capable of effectively capturing $CO_2$ in order to address this problem. The potential for $CO_2$ capture in solid-state materials such as zeolites, metal-organic frameworks, mesoporous silica, and carbon-based adsorbents has been studied.[2] Metal-organic frameworks (MOFs) are crystalline porous materials made from transition metal ions and connecting organic ligands, forming a robust, open crystalline structure. Due to their extremely high porosity, well-ordered and defined porous structures, and customizable chemical properties, MOFs are gaining significant interest for their potential uses in carbon capture and storage.[3] DFT computations are utilized to examine the $CO_2$ adsorption process within transition metal-doped MOF-5 {M-MOF-5 (M = Ni, Cu, Mn)} by monitoring the interactions between $CO_2$ and various binding sites of the doped MOF-5 structure. Through the optimization of both doped and undoped MOF-5 geometries, the objective is to compute the binding energy of metal atoms within the MOF-5 framework, the adsorption energy of CO2 molecules, and the extent of charge transfer between $CO_2$ molecules and the relevant adsorption systems. This work aims to explore the significant enhancement in the $CO_2$ adsorption capacity of MOF-5 facilitated by doping and a comparative analysis of different transition metal doped MOF-5 for their carbon capture efficiency.

#### References

[1] Mac Dowell N, Fennell PS, Shah N, Maitland GC. The role of CO2 capture and utilization in mitigating climate change. Nature climate change. 2017 Apr;7(4):243-9.
[2] Change NG. Global Surface Temperature| NASA Global Climate Change. Climate Change: Vital Signs of the Planet. 2023A A. First, B. Second and C. Third, Journal, 12 (2007) 345.
[3] Furukawa H, Cordova KE, O'Keeffe M, Yaghi OM. The chemistry and applications of metal organic frameworks. Science. 2013 Aug 30;341(6149):1230444

# Kinetic analysis of the non-isothermal decomposition of PEO10/25A/LiBOB polymer nanocomposite electrolytes

**MATKO ERCEG[1]*, IRENA KREŠIĆ[1], PETRA SKORIĆ[1]**

[1]Faculty of Chemistry and Technology, University of Split, Split, Croatia
*Corresponding author: e-mail: merceg@ktf-split.hr

**Keywords**: thermal decomposition, TGA, kinetic analysis

The melt intercalation method was used to prepare polymer nanocomposite electrolytes based on poly(ethylene oxide) (PEO10) ($\bar{M}_v = 1.000.000$), nanofiller - organically modified montmorillonite Cloisite 25A (25A) and lithium bis (oxalate) borate (LiBOB) salt (PEO/25A/LiBOB). Polymer nanocomposite electrolytes were obtained by mixing PEO10 with 25A in the indicated ratios (100/0, 90/10, 80/20, 70/30, 60/40 and 50/50) with the addition of LiBOB salt in an amount to meet the 1:8 ratio (Li:oxygen from PEO10). Thermogravimetric analysis (TGA) was performed in the temperature range 50-600 °C, at four heating rates (2.5; 5, 10 and 20 Cmin$^{-1}$), nitrogen atmosphere. Kinetic analysis of the thermal decomposition was used to reveal the influence of 25A and LiBOB on the thermal decomposition mechanism of PEO and to calculate the kinetic parameters of the thermal decomposition process. Calculations were performed using Netzch Professional Thermokinetic Software. The results show that thermal decomposition of PEO follows simple, one step decomposition mechanism while with the addition of 25A and LiBOB thermal decomposition follows complex, multi-step mechanism. Kinetic parameters of each decomposition step have been calculated.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

---

# Generalized interface reaction kinetic models for heterogeneous contracting processes

**LUIS A. PÉREZ-MAQUEDA[1]*, JUAN ARCENEGUI-TROYA[2], PEDRO E. SÁNCHEZ JIMÉNEZ[1], ANTONIO PEREJÓN[1,3]**

[1] Instituto de Ciencia de Materiales de Sevilla (CSIC-USE) Sevilla 41092, Spain
[2] Departamento de Electricidad y Electromagnetismo, Universidad de Sevilla, Sevilla 41012, Spain
[3]Departmento de Química Inorgánica, Universidad de Sevilla, Sevilla 41012, Spain
*Corresponding author: e-mail: maqueda@icmse.csic.es

**Keywords:** Heterogenous process; Interface kinetic model; Kinetics; Non-ideal kinetic model; Solid-state processes.

Kinetic analysis of heterogeneous processes implies getting reliable kinetic parameters that properly describe the process. Ideal kinetic models are used to gain insight about the process mechanism. These models are constrained by a number of assumptions rarely met in real systems. Thus, in the case of the commonly used contracting (or interface) kinetic models, For example, for the R2 ideal kinetic model, it is assumed a perfect cylindrical contraction in the radial direction, while contraction in the direction of the axis of the cylinder is not taken into consideration. Besides, for the R3 model, it is supposed contraction in all three directions of space for perfect spheres or cubes of identical dimensions. We have reanalysed contraction models considering different geometries, such as cylinders with different aspect ratios or rectangular cuboids and find mathematical equations for such processes. A new generalized interface reaction equation that covers all studied cases is presented. This new equation fits all studied cases including different geometries and particle size distributions. Presented equations are applied to real experimental data, providing a very accurate description of the studied processes.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Effect of Reaction Atmosphere on the Thermal Decomposition of Iron(III) acetylacetonate Leading to Iron Oxide Nanoparticles

**MANISHA CHAKRABORTY[1], ASHIS BHATTACHARJEE[1]***

[1]Department of Physics, Visva-Bharati, Santiniketan 731235, India
*Corresponding author: e-mail: ashis.bhattacharjee@visva-bharati.ac.in

**Keywords**: thermal decomposition, iron(III) acetylacetonate, kinetics

In 1991, Ismail [1] studied the thermal decomposition of iron(III) acetylacetonate in $N_2$ atmosphere. The decomposed material was identified as pure hematite. However, Ismail estimated only the average values of kinetic parameters but for most cases, the activation energy and reaction rate varied with the extent of conversion [2]. Hence, to estimate the conversion-dependent kinetic parameters, we have carried out a non-isothermal decomposition of iron(III) acetylacetonate for three different linear heating rates using thermogravimetry. Since the reaction atmosphere plays a big role in thermal decomposition [3], decomposition of iron(III) acetylacetonate in $O_2$ atmosphere was also carried out.

It is found that the thermal decomposition of iron(III) acetylacetonate is a three-step process in $N_2$ atmosphere whereas a six-step process under $O_2$ atmosphere. The kinetic parameters for all steps are estimated with the help of five integral iso-conversional methods. Master plot method is used to estimate the step-wise reaction mechanisms. Both activation energy and reaction rates are strongly dependent on the extent of conversion in both atmospheres. The average activation energies in $N_2$ atmosphere are found in the same range as those of Ismail's study for the first two steps, but for the third step the value estimated in present study is much higher than that of Ismail reported. The average values of reaction rate of this study are also higher compared to Ismail's study. Kinetic parameters of both atmospheres were compared. After evaluating the kinetic parameters, thermodynamic parameters are calculated for all steps under both atmospheres. From the results, the effect of the reaction atmosphere on thermal decomposition is clearly visible. The decomposed materials are characterized by powder XRD which confirmed the formation of iron oxide nanoparticles.

## References

[1] H. M. Ismail, *Journal of Analytical and Applied Pyrolysis*, 21 (**1991**) 315-326.
[2] M. Chakraborty, S. Kundu and A. Bhattacharjee, *Journal of Thermal Analysis and Calorimetry*, 148 (**2023**) 8915-8931.
[3] M. Chakraborty, S. Kundu and A. Bhattacharjee, *RSC Advances*, 13 (**2023**) 34972-34986.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermal stability of ammonia borane for alternative onboard hydrogen carrier

**Y . NAKAMURA[1], Y. IZATO[1], A. MIYAKE[2]***

[1] Graduate School of Environment and Information Sciences, Yokohama National University,
Yokohama 240-8501, Japan
[2] Institute for Multidisciplinary Sciences, Yokohama National University,
Yokohama 240-8501, Japan
*Corresponding author: miyake-atsumi-wp@ynu.ac.jp

**Keywords**: thermal stability, ammonia borane, hydrogen carrier

In order to extend the cruising range of fuel cell vehicles (FCVs), it is necessary to increase the onboard hydrogen capacity, and the use of ammonia borane, an alternative hydrogen carrier with a higher hydrogen density has been expected. However, ammonia borane is known to undergo an autocatalytic thermal decomposition accompanied by heat generation, expansion, and gas release, which may lead to container damage due to pressure rise inside the vehicle-mounted ammonia borane container. It is also known that the thermal decomposition mechanism of ammonia borane is extremely complex, and the reaction route varies greatly depending on the operated conditions.

The purpose of this study was to investigate the thermal stability of ammonia borane when installed in a vehicle. First, the thermal decomposition mechanism that may occur when ammonia borane is mounted on a vehicle was investigated using simultaneous TG-DTA with sample observation and heat and pressure measurements with Calvet type reaction calorimetry. Next, the self-accelerating decomposition temperature (SADT) of ammonia borane was estimated and compared with the required ambient temperature for onboard vehicle hydrogen carrier.

Based on the experimental results, it was found that the thermal decomposition of ammonia borane exhibits a nucleation-growth reaction, and the SADT was predicted as 329 K by kinetic analysis. And it is necessary to improve its thermal stability with gas release for the use of an alternative hydrogen carrier.

## References

[1] U. B. Demirci, *Int. J. Hydrogen Energy*, 42 **(2017)** 9978.
[2] U. B. Demirci, Inorg. *Chem. Front.*, 8 **(2021)** 1900.
[3] U. S. Department of Energy, DOE Technical Targets for Onboard Hydrogen Storage for Light Duty Vehicles, https://www.energy.gov/eere/fuelcells/doe-technical-targets-onboard-hydrogen-storage-light-duty-vehicles
[4] S. Basu et al., *J. Power Sources*, 196 **(2011)** 734.
[5] M. G. Hu et al., *Thermochim. Acta*, 23 **(1978)** 249.
[6] A. C. Stowe et al., *Phys. Chem. Chem. Phys.*, 9 **(2007)** 1831.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Water Vapor Effects on the Physico-Geometrical Consecutive Process of the Thermal Dehydration of Sodium Carbonate Monohydrate

**SHUNSUKE FUKUNAGA, MITO HOTTA, YUTO ZUSHI, NOBUYOSHI KOGA***

Grad. Sch. Humanities and Social Sciences, Hiroshima Univ., Higashi-Hiroshima, 739-8524, Japan
*Corresponding author: e-mail: nkoga@hiroshima-u.ac.jp

**Keywords**: thermal dehydration, kinetics, sodium carbonate monohydrate, humidity-controlled TG

The thermal dehydration of sodium carbonate monohydrate (SCM) exhibits a reversible feature and is significantly influenced by water vapor [1]. In addition, the thermal dehydration proceeds via a physico-geometrical consecutive process comprising the induction period (IP), surface reaction (SR), and phase boundary-controlled reaction (PBR) [2].

In this study, the effect of atmospheric and self-generated water vapor on the individual physico-geometrical reaction steps was investigated using the humidity-controlled thermogravimetry (HUM-TG, Rigaku). Based on the IP–SR–PBR model, the apparent rate constants of the individual reaction steps (i.e., $k_{\mathrm{IP}}$, $k_{\mathrm{SR}}$, and $k_{\mathrm{PBR}}$) were determined at various temperatures and water vapor pressures ($p(\mathrm{H_2O})$). The apparent $k$ values for each reaction step can be correlated as a function of temperature and $p(\mathrm{H_2O})$ with reference to the equilibrium pressure of the reaction ($P_{\mathrm{eq}}(T)$) [3,4].

$$k = A\exp\left(-\frac{E_{\mathrm{a}}}{RT}\right) h\left(p(\mathrm{H_2O}),\ _{\mathrm{eq}}(T)\right)$$

$$\text{with} \qquad h\left(p(\mathrm{H_2O}), P_{\mathrm{eq}}(T)\right) = \left(\frac{1}{p(\mathrm{H_2O})}\right)^{a}\left[1-\left(\frac{p(\mathrm{H_2O})}{P_{\mathrm{eq}}(T)}\right)^{b}\right], \qquad (1)$$

where $A$ and $E_{\mathrm{a}}$ are the Arrhenius parameters, and ($a$, $b$) are the constants characterizing the mechanistic feature of $p(\mathrm{H_2O})$ effect. Furthermore, the contribution of the self-generated $p(\mathrm{H_2O})$ ($p(\mathrm{H_2O})_{\mathrm{SG}}$) can be considered by introducing the effective $p(\mathrm{H_2O})$ ($p(\mathrm{H_2O})_{\mathrm{EF}}$) instead of the atmospheric $p(\mathrm{H_2O})$ ($p(\mathrm{H_2O})_{\mathrm{ATM}}$) in Eq. (1) [3,4].

$$p(\mathrm{H_2O})_{\mathrm{EF}} = p(\mathrm{H_2O})_{\mathrm{SG}} + d\cdot p(\mathrm{H_2O})_{\mathrm{ATM}} = c\cdot k + d\cdot p(\mathrm{H_2O})_{\mathrm{ATM}}, \qquad (2)$$

where ($c$, $d$) are the contributions of $p(\mathrm{H_2O})_{\mathrm{SG}}$ and $p(\mathrm{H_2O})_{\mathrm{ATM}}$, respectively. Based on Eqs. (1) and (2), the kinetics of the individual physico-geometrical reaction steps of the thermal dehydration of SCM was universally described over different temperatures and $p(\mathrm{H_2O})$ values.

**References**

[1] Y. Zushi, S. Iwasaki, N. Koga, *Phys. Chem. Chem. Phys.*, 24 (**2022**) 29827.
[2] Y. Zushi, S. Iwasaki, N. Koga, *Phys. Chem. Chem. Phys.*, 24 (**2022**) 15736.
[3] M. Hotta, L. Favergeon, N. Koga, *J. Phys. Chem. C.*, 127 (**2023**) 13065.
[4] M. Hotta, Y. Zushi, S. Iwasaki, S. Fukunaga, N. Koga, *Phys. Chem. Chem. Phys.*, 25(**2023**)27114.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Multistep Thermal Dehydration Kinetics of Geopolymer Pastes Prepared Using Different Active Fillers

**MANAMI SHINDO[1], AYA UEOKU[2], WAKANA OKAMURA[2], SHIN KIKUCHI[3], ATUSHI YAMAZAKI[2], NOBUYOSHI KOGA[1]***

[1] Grad. Sch. Humanities and Social Sciences, Hiroshima Univ., Higashi-Hiroshima 739-8524, Japan
[2] School of Creative Science and Engineering, Waseda Univ., Shinjuku 169–8555, Japan
[3] Fast Reactor Cycle System Research and Development Center, Japan Atomic Energy Agency, Higashi-Ibaraki 311-1393, Japan
*Corresponding author: e-mail: nkoga@hiroshima-u.ac.jp

**Keywords**: thermal dehydration, geopolymer, kinetic deconvolution analysis

Geopolymer pastes exhibit multistep thermal dehydration/decomposition [1,2]. Regardless of the samples prepared using different active fillers including metakaolin (MK), fly ash (FA), and blast furnace slag (BFS), two-step thermal dehydration occurred by partially overlapping, in which the first and second reaction steps were accompanied by the evolutions of water vapor and water vapor–$CO_2$, respectively (Fig. 1). In this study, the kinetic features of the partially overlapping two-step dehydration processes were investigated at different atmospheric water vapor pressures ($p(H_2O)$) to reveal the water vapor release behavior from the geopolymer pastes characterized by a lower water content.

The kinetic data of the partially overlapping two-step dehydration process were extracted from TG–DTG curves recorded under nonisothermal conditions at various $p(H_2O)$ values using the mathematical deconvolution analysis [3]. Further, the multistep kinetics was analyzed using the kinetic deconvolution analysis [3]. Irrespective of the samples, both component reaction steps exhibited diffusion-controlled reaction behaviors. The first reaction step was significantly influenced by the atmospheric $p(H_2O)$, whereas the second reaction step was less sensitive to that. The kinetic results are detailed in this presentation.

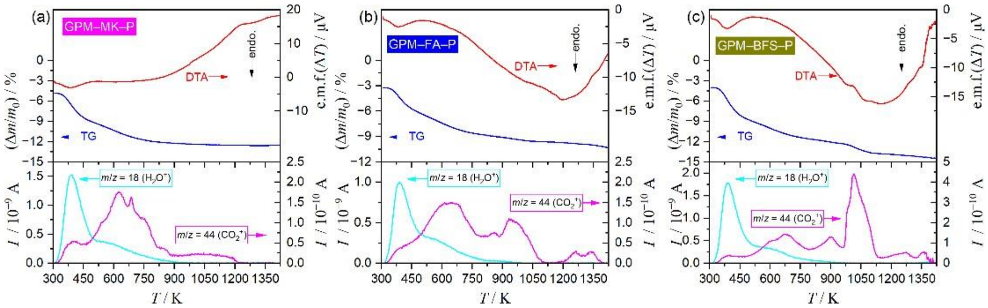


Fig.1: TG/DTA–MS of the geopolymer pastes based on (a) MK, (b) FA, and (c) BFS.

## References

[1] R. He, N. Dai, Z. Wang, *Adv. Civil Eng.*, 2020 **(2020)** 7532703.
[2] L. Kljajevic, et. al, *gels*, 8 **(2022)** 333.
[3] N. Koga, Y. Goshi, S. Yamada and L. A. Pérez-Maqueda, *J. Therm. Anal. Calorim.*, 111 **(2013)** 1463–1474.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Enhancing Thermal Analysis Precision: Exploring Isoconversional Methods for Accurate Data Evaluation

**E. TARANI, K. CHRISSAFIS***

Department of physics, Aristotle University of Thessaloniki, Thessaloniki 54124, Greece
*Corresponding author: e-mail: hrisafis@physics.auth.gr

**Keywords**: isoconversional methods, data quality, activation energy, kinetic analysis

This study examines the importance of isoconversional techniques in thermal analysis and their crucial role in assessing the accuracy of experimental findings. It investigates the thermal degradation of polylactic acid tannin nanocomposites and the non-isothermal crystallization of poly(ethylene 2,5-furandicarboxylate) carbon nanotube nanocomposites. Four commonly used methods were applied to calculate activation energy ($E_\alpha$) and pre-exponential factors relative to the conversion degree. The evaluation of error bars further helped assess calculation precision. The discussion addresses the influence of temperature variations on data integrity, emphasizing their significant impact on results. The precision of these measurements relies not only on temperature and material quality but also on the chosen mathematical technique for baseline deduction. Isoconversional methods demonstrate distinct behaviors, underscoring the importance of accurate data and analytical methods [1]. Temperature variations not only affect $E_\alpha$ but also alter curve shapes, with error bars showing increased sensitivity to even minor temperature shifts. Errors in baseline deduction might lead to inaccurate results and affect $E_\alpha$ estimation [Fig. 1]. The study emphasizes the importance of strict quality control for reliable and accurate kinetic analysis.

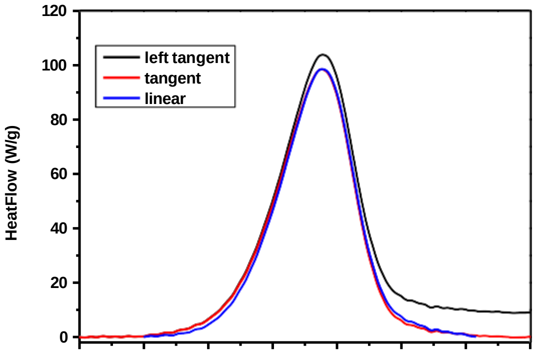


Fig. 1: Heat flow curves versus temperature after baseline subtraction using tangential, left tangential and linear curve subtraction methods

## References

[1] S. Vyazovkin, K. Chrissafis, M.L. Di Lorenzo, N. Koga, M. Pijolat, B. Roduit, N. Sbirrazzuoli and J.J. Sunol, *Thermochim. Acta*, 590 (**2014**) 1-23.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Enhancing Green $H_2$ Generation: The Role of Oxide-Nitride Interface Based Electrocatalysts

**ARPAN TEWARY[1]***

[1]Rajiv Gandhi Institute of Petroleum Technology Jais, Amethi-229304, India
*Corresponding author: e-mail: 20bs0012@rgipt.ac.in

**Keywords**: Green $H_2$, Oxide-nitride interphase, Hydrogen evolution, Sustainability

Water electrolysis is a promising pathway for sustainable green hydrogen generation, and the development of efficient and stable electrocatalysts is crucial for this process. Oxide-nitride interfaces have emerged as a powerful platform for electrocatalysis due to their unique electronic structures, enhanced surface properties, and stability under electrochemical conditions. The combination of oxides and nitrides at the interface can create a synergistic effect that improves catalytic activity and durability. The oxide component possibly provides strong electrochemical activity, while the nitride phase offers active sites with high catalytic efficiency for hydrogen evolution reactions (HER). This interface engineering approach can enhance charge transfer, reduce energy barriers, and improve overall catalytic performance. Tuning the composition, morphology, and electronic properties of oxide-nitride interfaces can significantly increase their activity in HER. Moreover, these materials exhibit remarkable stability in alkaline and acidic electrolytes, making them versatile for various water-splitting technologies. Herein we discuss the design principles, synthesis strategies, and electrochemical performance of oxide-nitride interface-based electrocatalysts. By focusing on recent advancements and the underlying mechanisms that govern their activity, we aim to provide insights into the development of next-generation electrocatalysts for green hydrogen production. Our findings suggest that optimizing oxide-nitride interfaces could lead to more efficient and sustainable hydrogen generation processes, contributing to the broader goal of renewable energy adoption and reducing carbon footprints.

**References**

[1] Shao, M., Chang, Q., Dodelet, J. P., Chenitz, R. Recent advances in electrocatalysts for oxygen reduction reaction. *Chem. Rev.* **2016**, 116, *6*, 3594–3657.

[2] Zhu, Y., Lin, Q., Zhong, Y., Tahini, H. A., Shao, Z., Wang, H., Metal oxide-based materials as an emerging family of hydrogen evolution electrocatalyst electrocatalysts *Energy Environ. Sci.*, **2020**,13, 3361-3392.

[3] Tian, L., Zhao L., Song, M., Li, J., Recent progress in water-splitting electrocatalysis mediated by 2D noble metal materials *Nanoscale,* **2021**, 13, 12088-12101.

# Nanoporous Samarium and Cerium-Based Metal-Organic Frameworks for Enhanced Photocatalytic Water Splitting

**HARIKRISHNA RB[1,2,3], DEEP LATA SINGH[1,3], SUNDARARAJAN T[2,3], RANGA RAO G[1,3*]**

[1]Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036, India
[2]Department of Mechanical Engineering, Indian Institute of Technology Madras, Chennai-600036, India
[3]DST Solar Energy Harnessing Centre, Indian Institute of Technology Madras, Chennai-600036, India
*Corresponding author: e-mail: grrao@iitm.ac.in

**Keywords**: Metal-organic framework, photocatalysis, water splitting

Lanthanide metal-organic frameworks (MOFs) are promising for photocatalytic water splitting, turning water into hydrogen and oxygen using sunlight. These materials uniquely combine properties ideal for this purpose. Lanthanide ions, with their specific electronic configurations, enable efficient light absorption and energy transfer. The porous, adjustable structure of MOFs is great for incorporating lanthanide ions and other elements, enhancing photocatalytic effectiveness. These ions can act as sensitizers, broadening the material's light absorption range for better solar energy usage. It also serves as redox centers, aiding charge separation and transfer in water splitting. The MOF's well-defined pore structure facilitates reactant and product diffusion, boosting photocatalytic activity. Our research focused on samarium and cerium ions with 5-nitroisopthalic acid as a ligand, showing strong coordination and maintaining structural stability, with promising gas chromatography results.

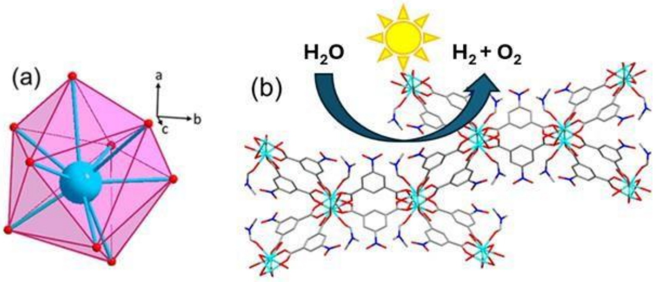


Fig. 1: (a) Coordination of ligand around metal ions and (b) 2D representation of the crystal.

**References**
[1] J. Sowik, T. Grzyb, G. Trykowski, T. Klimczuk, et al., International Journal of Hydrogen energy, 47, 2022, 16065-16079.
[2] H. Yang, L. Jia, Z. Zhang, B. Xu et al., Jouranal of Catalysis, 405, 2022, 74-83.
[3] S. Navalon, A. Dhakshinamoorthy, M. Alvaro et al., Chemical Reviews, 123, 2023, 445-490.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Kinetic study of the dissociation of $[Co(tpy)_2]^{2+}$: Comparison between AOT/Heptane and CTAB/Chloroform/Hexane reverse micellar environments.

**B. LEELA KUMARI [1], P. SHYAMALA [2*], K.V. NAGALAKSHMI [3]**

[1]Department of Chemistry, St.Joseph's college for women , Visakhapatnam - 530004, Andhra Pradesh, India.
[2]Department of Chemistry, Andhra University, Visakhapatnam - 530003, Andhra Pradesh, India.
[3]Department of chemistry, Gayatri Vidya Parishad College of Engineering (A), Visakhapatnam-530048, Andhra Pradesh, India.
*Corresponding Author: shyamalapulipaka06@gmail.com

**Keywords**: $[Co(tpy)_2]^{2+}$, CTAB(cetyltrimethylammonium bromide), AOT , reverse micelles and waterpool

The kinetic study of dissociation of $[Co(tpy)_2]^{2+}$was carried out in two distinct reverse micellar environments, AOT/heptane and CTAB/hexane/chloroform. The reaction rates were significantly accelerated within the reverse micelles compared to aqueous medium, where the reaction was notably slow and incomplete{$k_{CTAB} = 6.9\times10^{-5} s^{-1} < k_{AOT} = 31.5\times10^{-3} s^{-1}$}. The enhanced reaction rate in reverse micelles was attributed to the lower dielectric constant of water present in the reverse micelles which increases with the value of W. Kinetic profiles were investigated as a function of parameters like concentration of surfactant and amount of water present in the core of reverse micelles, $H_2O$]/[surfactant] {= W}. Analysis revealed that, the rate of reaction decreases with increasing the ratio of [$H_2O$]/[surfactant] {= W} in both the micellar media. The reaction rate was observed to vary with the concentration of the anionic surfactant (AOT) and but independent of the concentration of the cationic surfactant (CTAB). The dependence of rate of reaction on surfactant concentration could be explained on the basis of electrostatic interactions between electro positively charged complex$[Co(tpy)_2]^{2+}$and charge of micellar interface.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Kinetics on the Thermal Degradation of Polyimide

**SHUTO YAMADA[1]*, KENSHIRO HIRAI[1], MASAHIRO TSUCHIYA[1],
NOBUYOSHI KOGA[2]**

[1] Department of Applied Chemistry, National Defense Academy of Japan, Kanagawa 239-8686, Japan
[2] Graduate school of Humanities and Social Sciences, Hiroshima University, Hiroshima 739-8524, Japan
*Corresponding author: e-mail: shtymd@nda.ac.jp

**Keywords**: thermal degradation, kinetic analysis, deconvolution, polyimide

Aromatic polyimides are used in the fabrication of microelectronic devices because of their excellent thermal, chemical and mechanical properties due to the units of aromatic and imide rings in the chain backbone. A representative aromatic polyimide is poly(4,4’-oxydiphenylene pyromellitimide) which is well known as Kapton®† film. The thermal behavior of Kapton is widely studied to predict the lifetime and develop new heat-resistant plastics. The thermal degradation of Kapton occurs in solid state generating various gaseous products, and exhibits multistep kinetic behavior [1, 2]. In previous studies, the kinetic models for the thermal degradation of Kapton has been discussed on the basis of assumptions, including single-step approximation, that is, the reaction regulated by a single rate-determining step in the main mass-loss step.

In this study, the kinetic behavior of the thermal degradation of Kapton was investigated based on the mass-loss curves recorded under linear non-isothermal conditions at various heating rates. The thermal degradation of Kapton proceeded in a smooth single step mass-loss process. However, the results of isoconversional kinetic analysis indicated three distinguishable ranges with regard to the constancy of the apparent activation energy. The gaseous products during the thermal degradation of Kapton, as measured by pyrolysis gas chromatography/mass spectrometry, were roughly divided into three categories based on differences in degradation reactions (cleavage of imide rings and ether bonds, and the degradation reaction of intermediate degradation product).

The results of the kinetic deconvolution analysis [3] indicated that the thermal degradation of Kapton is a partially overlapping process comprising three physico-chemical reaction processes, represented as *n*th-order reactions. A change in the chemical process during the thermal degradation of Kapton is discussed as one of the possible causes for the multi-step kinetic behavior of the overall reaction.

† Kapton is a registered trademark of affiliates of DuPont de Nemours, Inc.

**References**

[1] L. Li et al., *Polym. Degrad. Stab.*, 84 **(2004)** 369.
[2] A. C. Lua et al., *Polym. Degrad. Stab.*, 91 **(2006)** 144.
[3] N. Koga et al., *J. Therm. Anal. Calorim.* 111 **(2013)** 1463.

# Correlation between crystal structure parameters with optical, electronic, luminescent, and magnetic parameters of barium hexaferrite nanomaterials at controlled thermal temperature

**ZEESHAN HASMI[1], RAKESH KUMAR SINGH[1], NISHANT KUMAR[1], MONALISA[1], R. K. VERMA[2,3,4]**

[1]Aryabhatta Knowledge University, Patna: 800001
[2] University Department of Chemistry, Magadh University, Bodh Gaya 824234, India
[3] Patna University, Patna-800005
[4] Munger University, Munger-811201
*Corresponding author: e-mail: rakeshsinghpu@gmail.com

**Keywords**: thermal analysis, DSC, citrate precursor, optical properties

The citrate precursor sol-gel method is used to create M-type barium hexaferrite ($BaFe_{12}O_{19}$)[1]. Our earlier report has been revisited with extra inputs. The hexagonal crystal structure with P63/mmc space group of the synthesized nanomaterials was confirmed by the X-ray spectra and was found to be present in a pure phase. In the hexaferrite nanomaterials, the crystallite size and lattice strain are determined using the Williamson-Hall plot. Due to induced lattice strains in the samples, the lattice parameters (a) and (c) exhibit considerable increases. The FTIR spectrum effectively supports the XRD findings. The direct and indirect band was found to decrease from 2.32 eV to 1.81 eV and 3.41 eV to 3.18 eV respectively. Zeta potential measurements show that the stability increases with the annealing temperature. With annealing, the magnetic properties of nanomaterials are improved, with notable rise in magnetization (26.91-71.74 emu/g) and retentivity (37.24-72.25 emu/g). Coercivity dramatically rises from 161.33 to 4563 Gauss. The present study investigates the relationship between induced lattice strain and enrichment of structural, optical and magnetic characteristics at various annealing temperatures

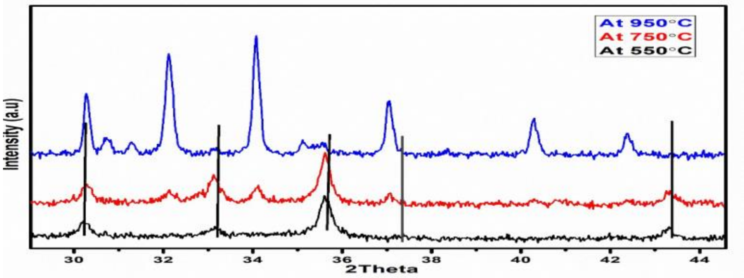


Fig. 1 : Shift in prominent peak and planes [104] and [108] intensity of intermediate phases (-Fe2O3) with annealing temperature

**References**

[1] R. K. Verma, R. K. Singh, A. Narayan, L. Verma, A.K. Singh, A. Kumar, P.K. Pathak, A. K. Aman. Low-temperature synthesis of hexagonal barium ferrite (BaFe12O19) nanoparticles by annealing at 450 °C followed by quenching. J Therm Anal Calorim.2017;129: 691–9.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Exploring the Protective Effects of Surfactants against Corrosion: A Comprehensive Review

**MANOJ KUMAR ADHIKARI[1], CHANDRADIP KUMAR YADAV[2*], RICHA GUPTA[1], JASANA MAHARJAN[3], AMAR PRASAD YADAV[1], AJAYA BHATTARAI[4*]**

[1]Central Department of Chemistry, Tribhuvan University, Nepal
[2]Amrit Science Campus, Tribhuvan University, Nepal
[3]Padam Kanya Multiple Campus, Tribhuvan University, Nepal
[4]Mahendra Morang Aadhrash Multiple Campus, Tribhuvan University, Nepal
*Corresponding author: e-mail: Chandradip2y@gmail.com/bkajaya@yahoo.com

**Keywords**: Anti-corrosive material, critical micelle concentration, surfactants, aggregation, Protective methods

Concerns has long existed over the impact of corrosion on the structural integrity of metal surfaces. Chemical corrosion inhibitors are frequently used in manufacturing and processing processes. However, the task at hand involves creating a novel class of corrosion inhibitors to safeguard environmentally friendly materials in a variety of scenarios. Surfactants are a highly affordable, readily available, and environmentally friendly choice for corrosion inhibitors. This review article's objective is to outline surfactants' capacity to prevent corrosion on various metal surfaces. The properties of multiple kinds of surfactants and their possible applications have also been discussed. This review article also discusses a number of other factors, including the effect of surfactant content, temperature, the underlying process of corrosion inhibition, and the manner of adsorption.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

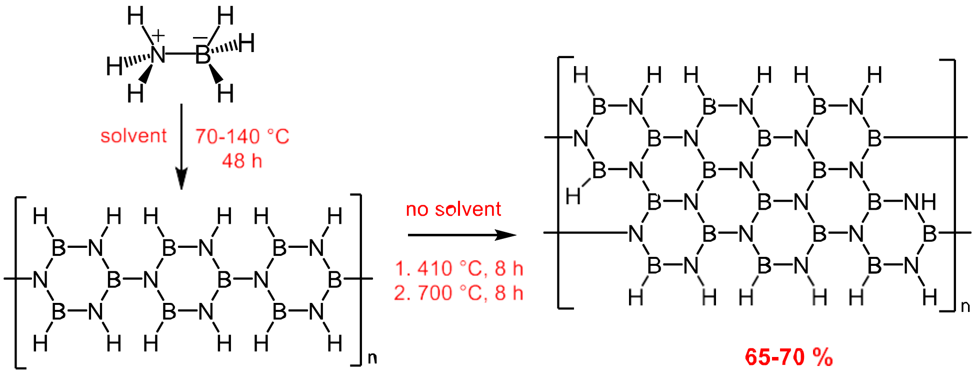
# Polyborazylene characterization: Determination of subsequent polymerization steps by DTA analysis

**VITEZSLAV ZIMA[1], PETR KNOTEK[2], ROMAN KEDER[3], NADEZDA MALKOVA[3]**

[1] SYNPO a. s., Pardubice, Czech Republic
[2] University of Pardubice, Faculty of Chemical Technology, Pardubice, Czech Republic
[3]Katchem spol. s r. o., Prague, Czech Republic
Corresponding author: keder@katchem.cz

**Keywords:** polyborazylene, DTA, borazine, hexagonal boron nitride

Polyborazylene is fine white powder oligomer, its molecular structure lies between monomeric structure of borazine and final polymeric structure of hexagonal boron nitride. Its molecular structure and physical properties depend on the method of synthesis, precisely on the reaction temperature and reaction time. These polyborazylene derived materials can be used as fillers in new types of polymer composite materials. It is presumed that these materials treated at temperatures of 700 °C and higher can form a kind of precursors of hexagonal boron nitrides (*h*-BN).



DTA analysis was primarily used to determine of the degree of polymerization. The amount of hydrogen released was observed. Thanks to DTA analysis, it was also found out that the reaction solvent is relatively strongly intercalated between the polyborazylene layers.

This project is financially supported by the Czech Technology Agency (No. FW06010094).

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Specific heat capacity measurement of silica glass by differential scanning calorimeter

**HARUKA ABE**[1]*

[1]National Metrology Institute of Japan (NMIJ), National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki 3058563, Japan
*Corresponding author: e-mail: abe-haruka@aist.go.jp

**Keywords**: Specific heat capacity, DSC, Reference material,

Silica glass is a material with high purity, high transmittance, excellent heat resistance, and chemical durability. Due to these characteristics, it is used in various experimental components such as optical filters, lenses, etc. Furthermore, because it is very stable over a wide temperature range, it is also used as the reference material such as NMIJ CRM5809a [1] for thermal diffusivity, NMIJ CRM5802a for thermal expansion, and as a thin film substrate of NMIJ CRM5808-a and 5810-a for thermal diffusivity.

In this study, the specific heat capacities of fused and synthetic quartz were measured in detail using a differential scanning calorimeter (DSC). In addition, the silica glass was also measured for the substrate material for NMIJ CRM 5810-a by the DSC at room temperature. The uncertainty of the DSC measurement will be presented and discussed.

**References**

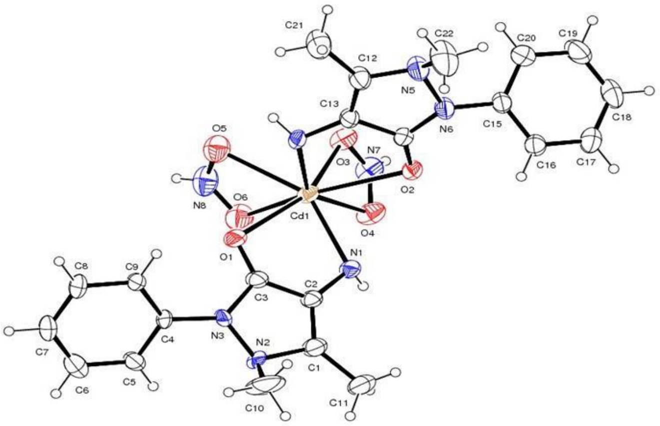
[1] Mu Li, M. Akoshima, International J. Thermal Science, 165 (2021) 106955-1.

# Green route Synthesis, Spectral characterization and Crystal structure of [Cd(4-AAP)$_2$(NO$_2$)$_2$]

**K. RAJASEKAR[1*], R. SELVARANI[2] AND C. VEERAVEL[3]**

[1]PG & Research Department of Chemistry, Govt. Arts College, Ariyalur-621713, Tamil Nadu, India.
(Affiliated to Bharathidasan University, Tiruchirappalli-620024)
[2]Department of Chemistry, Government Arts and Science College, Tittagudi, Tamil Nadu, India
[3]Meenakshi Ramasamy Engineering College, Thathanur, Tamil Nadu, India
*Corresponding author: e-mail: yokkesh111@gmail.com

The cobalt metal chelate was synthesized under microwave irradiation (green technology) and the structural aspects of the complex were determined from elemental analysis, conductance measurement, FT-IR, NMR spectra and single crystal X-ray diffraction analysis. The spectral and X-ray diffraction studies of the complex indicate that the crystal system is monoclinic with the P21/n space group. The cadmium ion in this compound is coordinated with two bidentate modes of both nitrite groups and 4-aminoantipyrine ligands with extended coordination. The nitrite ions and 4-aminoantipyrine molecules are bidentate to the metal ion and form four member chelate rings. The geometry of the complex is distorted dodecahedron.



# An analytical review of the current status and challenges in the development of inorganic phase change materials for thermal energy storage

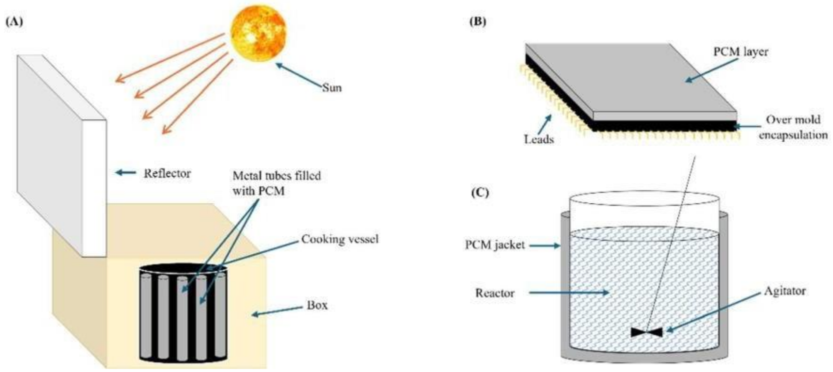
SOMYA DEEP DEY[1], DEBABRATA PANDA[2], KRUNAL MADHUKAR GANGAWANE[1]

[1]Department of Chemical Engineering, Indian Institute of Technology, Jodhpur 342030, India
[2]Department of Chemical Engineering, NIT Rourkela, Odisha 769008, India
*Corresponding author: e-mail: krunalg@iitj.ac.in

Keywords: Phase change materials, inorganic salt hydrates, thermal energy storage, solar energy, heat transfer augmentation

Latent heat thermal energy storage (LHTES) systems are one of the eminent and efficient solutions of storing thermal energy at a constant phase change temperature. A major challenge in LHTES is the proper selection of phase change materials (PCMs) in target applications such as solar cookers, semiconductors, reactors, batteries, etc. As compared to organic PCM, inorganic PCM have drawbacks of corrosion potential, sub-cooling, flammability, and phase separation; however, some methodologies to minimize these drawbacks (core-shell encapsulation, shape-stabilization, electroplating, inverse Pickering emulsion) along with higher thermal conductivity, and higher TES capacity in medium to higher range of temperature applications precedence its applicability. This study explored a detailed review of inorganic PCMs in terms of research outcome and technological advancement while focusing on the capability of providing solutions in TES [1]. A detailed thermal characterization study focusing on long term stability, thermal cycling performance, and heat transfer augmentation are also discussed in the context of heat and storage capacity properties [2] of the salt hydrates.

GRAPHICAL ABSTRACT



**References:**

[1] B. Zalba, J. M. Marín, L. F. Cabeza, and H. Mehling, *Appl Therm Eng*, 23(3) (**2003**) 251–283.

[2] S. Agarwala and K. N. Prabhu, *J Energy Storage*, 46 (**2022**) 103865.

**T4- PP 01**

# Preparation and characterization of microencapsulated antimicrobial insock/footbed for foot comfort

**K. AMBIKA[1]*, M. AKSHAYARAMAN [2], Dr MATHIVANAN S[3]**

[1]Shoe and Product Design, Development Center, CSIR-CLRI, Chennai-600020, India
[2] Shoe and Product Design, Development Center, CSIR-CLRI, Chennai-600020, India
[3] Shoe and Product Design, Development Center, CSIR-CLRI, Chennai-600020, India
*Corresponding author: e-mail: ambika@clri.res.in

**Keywords**: Antimicrobial, Melaleuca alternifolia, Tea tree oil, Lemon Oil, Cinnamon oil, Insock/Footbed, SEM, FTIR, DLS Spectrophotometry.

The aim of this work is to prepare a microencapsulated antimicrobial agent for footwear insock/footbed against microbial overgrowth on human's foot. Melaleuca alternifolia (Tea tree oil), Lemon oil and Cinnamon Oil loaded microcapsules were used for this antimicrobial study purpose. Microencapsulation is one of the proven productive methods for prevention of these natural biocides from moisture, interactions, heat, pressure and exposure to oxygen. Primarily, this technique reduces the evaporation rate of the active core materials. Microcapsules were prepared by in-situ polymerisation method from different ratio of emulsion formulation. Microcapsule characterization, such as particle size, morphology, chemical properties, encapsulation yield, encapsulation efficiency, oil content were determined using SEM, FTIR, DLS spectrophotometry. Stability of the emulsions was determined by antimicrobial test methods. The prepared microcapsule was incorporated into various footwear materials like leather, fabrics, and polymers. The physical changes in the insock/footbed material, diffusion of emulsion in insock/footbed material, determination of release quantity of core material at foot temperature, pH and foot warm conditions were also elucidated. Microbiological tests and in vitro release studies were also analysed for the prepared microencapsulated insock/footbed materials. Microencapsulated antimicrobial agent coated footwear material has higher functional efficiency against the microorganism's growth.

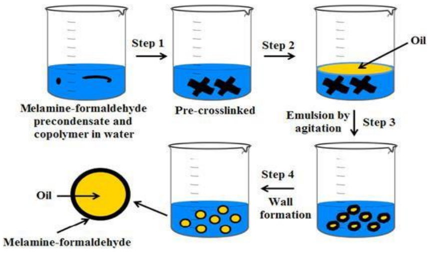


Fig. 1 : Microcapsule preparation

**References**

[1] Ajmed, J., Zulifar, A., Tanveer, H, *J.Microencapsulation.*, Faisalabad ,2014. Online 1-8.
[2] Buket, Y., Huseyin, A Johnson *Mattehey Techol. Rev*,Bornova-IzmirTurkey,2020,Vol64, Issue 4
[3] Du, L., Li, T., Wu, S., Zhu, H., Zou, Y. *Royal Society of Chemistry*,China, 2019, 9: 2244-2251.

# Crystallization kinetics to achieve Stoichiometric Combeite ($Na_2Ca_2Si_3O_9$) and Silicorhenanite ($\beta$-$Na_2Ca_4(PO_4)_2SiO_2$) Single Phasic Bioactive Glass System

**<u>VIJAYAKUMARI.S</u>, BALAKUMAR.S***

National Centre for Nanoscience and Nanotechnology, University of Madras, Chennai – 600025, India
*Corresponding author: e-mail: balasuga@yahoo.com

**Keywords**: thermal analysis, TG-DTA, kinetic models, activation energy.

The great versatility and suitability of bioactive glass in the field of medicine led to the advancement of many clinical products for the well-being and rehabilitation of patients. One of the major drawbacks focused in this study is the crystallization of the bioactive glasses. The crystallization or partial crystallization of the bioactive glasses is reported to decrease the bioactivity of the material at an increasing temperature during heat treatment. The reports show that low-temperature sintering of silicate glasses results in a sodium-rich phase whereas higher-temperature sintering yields a phosphate-rich phase[1,2].

Combeite ($Na_2Ca_2Si_3O_9$), a silica-rich crystallographic phase, and Silicorhenanite ($Na_2Ca_4(PO_4)_2SiO_4$), a phosphate-rich crystallographic phase form during heat treatment of bioactive glass compositions and play a major part in deciding the properties of the biomaterials. Determining crystallization kinetics is one of the appreciable routes to achieve the desired phase and predict the bioactivity of the material. From the study, it is found that sol-gel derived bioactive glasses require 141.49 kJ/mol to form the Combeite phase and only 81.95 kJ/mol of activation energy to form the Silicorhenanite phase. The obtained results are lower than the energy required for crystalline hydroxyapatite and offer a unique material for rapid bioactivity.

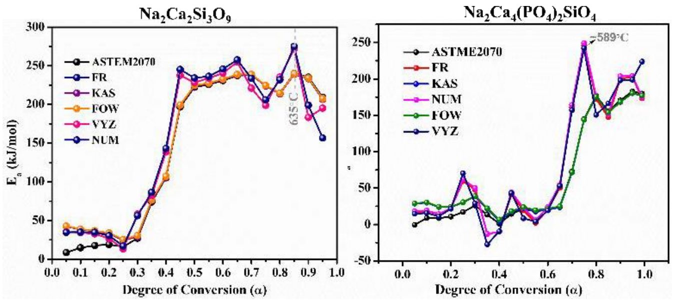


Fig. 1 : α Vs $E_a$ curve of (a) Combeite - $Na_2Ca_2Si_3O_9$ and (b) Silicorhenanite - $Na_2Ca_4(PO_4)_2SiO_4$ crystallographic phases

## References

1 M. Magallanes-Perdomo, S. Meille, J.-M. Chenal, E. Pacard and J. Chevalier, *Journal of the European Ceramic Society*, 2012, **32**, 2765–2775.

2 L. Lefebvre, J. Chevalier, L. Gremillard, R. Zenati, G. Thollet, D. Bernache-Assolant and A. Govin, *Acta Materialia*, 2007, **55**, 3305–3313.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

---

# Separation of 5-HMF from the Ionic Liquids Using Phenolic Solvents Using Molecular Dynamics Simulations

**SWETA JHA [1]*, PRAVEENKUMAR SAPPIDI[2]**

[1] Department of Chemical Engineering, Indian Institute of Technology Jodhpur 342037, India
[2] Department of Chemical Engineering, Indian Institute of Technology Jodhpur 342037, India
*Corresponding author: e-mail: p22ch007@iitj.ac.in

**Keywords**: MD Simulation, Furfural, Ionic liquids, thermodynamics, alkylated phenolic solvent.

To achieve a sustainable future to reduce global warming, there is a significant need for renewable energies such as solar, wind, geothermal, hydrothermal, and bioenergy.[1] Bioenergy derived from biomass has great attributes such as its abundant nature, and non-toxic to the environment. The feedstocks that are derived from the lignocellulosic biomass (LCB) are tangible to decrease greenhouse gases and found immense applications in the field of the production of fuels and value-added chemicals etc.[2, 3] As per the Department of Energy, USA, 5-hydroxy-methyl-furfural (5-HMF) and other furfurals can be used in refineries and help generate biorefinery as well as green polymers, solvents, fungicides, and a range of chemical products.[4] Ionic liquids (ILs) are shown to be promising and very efficient in synthesizing 5-HMF from fructose. However, there is still a great challenge in separating the 5-HMF from the ILs. Various organic solvents are effective in separating 5-HMF from the ILs. However, 5-HMF can be extracted from ILs using organic solvents (hydrogen bond donors property) shown promising for the highly efficient extraction of 5-HMF.[5] In this presentation, we aim to investigate various phenolic solvents that help in the effective separation of 5-HMF from ILs. We present various structural properties, interactions, dynamic properties, and separation thermodynamic properties. Our results show that the effective separation depends upon the role of the hydrophobicity of the solvent (4BP, 4PP, 4EP, 4MP). The self-diffusivity (D) of 5-HMF shows a decrease with an increase in the methyl group on the phenol. Due to the variation in the alkyl group on the phenols the oxygen atom of 4MP solvent shows a strong interaction with Solvent-$[BF_4]^-$ and solvent-$[BMIM]^+$. Interestingly we see higher mobility of the 5-HMF molecule due to the weak intermolecular interactions in the 4MP, thereby less solvation as seen from the solvation free energy calculations. Overall results obtained in this work were shown promising for the understanding of the complex interactions between furfural-based compounds and ILs for the separation of pure 5-HMF using an alkylated phenolic solvent.

## Reference

(1) Ellabban, O.; Abu-Rub, H.; Blaabjerg, F. *Renewable and sustainable energy reviews* **2014**, *39*, 748-764.
(2) Pauly, M.; Keegstra, K. *Current opinion in plant biology* **2010**, *13* (3), 304-311.
(3) Gupta, S.; Haider, M. A. In *Hydrocarbon Biorefinery*, Elsevier, 2022; pp 409-430.
(4) Bozell, J. J.; Petersen, G. R. *Green chemistry* **2010**, *12* (4), 539-554.
(5) Wang, H.; Cui, J.; Zhao, Y.; Li, Z.; Wang, J. *Green Chemistry* **2021**, *23* (1), 405-411.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Optical properties of $Dy^{3+}$ doped tin borophosphate glass for radiation shielding applications

**A. INCELET JOBIKHA[1], K.PRADHEESHA[1], K.ANU JOHN[1], A.PAUL DHINAKARAN[1] ,P.VINOTHKUMAR[1*]**

[1]Department of Physics, Saveetha Engineering College, Thandalam, Chennai – 602105, India.
*Corresponding author: e-mail: newtonphysics329@gmail.com

**Keywords**: Glass, Gamma Ray, Borophosphate Glass, Photoluminescence, FTIR.

This study investigates the radiation shielding properties of $Dy^{3+}$ doped tin borophosphate glass with the composition ($40B_2O_3$-$30P_2O_5$-$10LiCO_3$-5AgO-3MgO-$5SnO_2$-6ZnO-$1Dy_2O_3$) fabricated using the melt quenching method. The glass composition was confirmed by powder X-ray diffraction (XRD), while Fourier-transform infrared (FTIR) and Raman spectroscopy were employed to identify functional groups within the glass. Optical properties, including the refractive index and optical band gap energy, were analyzed through UV-Vis spectroscopy. The photoluminescence characteristics of the $Dy^{3+}$ doped glass were investigated to understand its luminescent behavior. Mechanical properties were evaluated using a Vickers microhardness tester. The elemental composition was determined by Energy Dispersive X-ray Spectroscopy (EDAX). Radiation shielding performance, including parameters such as mean free path (MFP), mass attenuation coefficient (MAC), half value layer (HVL), and effective atomic number (Zeff), was assessed using Phy-X software. The results indicate that the $Dy^{3+}$ doped tin borophosphate glass has promising properties for radiation shielding applications.

**References**

[1] Takebe H., Harada T., Kuwabara M, J., Non-Cryst. Solids (2006) 352 ,709.
[2] Bingham A., Hand. R. J., Forder S.D., Lavaysierre A., Deloffre F., Kilcoyne S., H,Yasin I., Phys Chem. Glasses: Eur. J. Glass Sci.Technol. B.2006 4, 313.
[3] Marotta A., Buri A., Branda F., Pernice P., Aronne A., J. Non-Cryst. Solids (1987) 95&96,593.

T5- PP 02

# Superhydrophobic nanocomposites for coating leather and other surfaces

**D.R. SANGEETHA, BHUVANESWARI T S, N NISHAD FATHIMA***

CSIR-CLRI, Chennai-600020, India
*Corresponding author: e-mail: nishad@clri.res.in

**Keywords:** Superhydrophobicity; Leather finishing; Self-cleaning, Oil-water separation; Hybrid nanocomposite.

Superhydrophobic coatings have attracted significant attention due to their long term superhydrophobicity, oil-water separation, anti-fouling, self-cleaning properties and so on. In our study, we have synthesized a superhydrophobic hybrid nanocomposite using hexamethyldisilazane (HDMS)-modified $SiO_2$ with acrylic resin, coupled with γ-aminopropyl triethoxy silane (γ-APS). The prepared material was characterized by FT-IR, TGA, particle size analyser, FE-SEM and the covalent network of HMDS, γ-APS with $SiO_2$ was confirmed. The material was coated on various surfaces and tested for stability under different chemical and thermal conditions. The contact angle measurement was done on different chemical environment and contact angle above 150° was obtained.

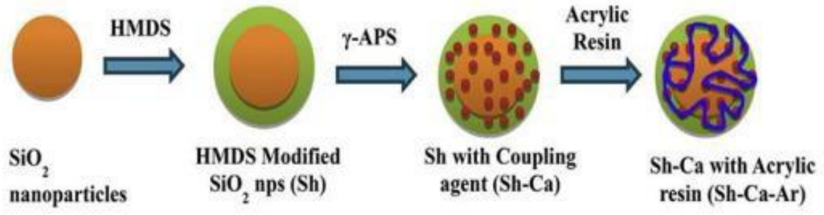


Fig. 1: Schematic representation of hybrid nanocomposite formation

We are presently exploring its application for developing superhydrophobic leather so that leather can be protected from water damage, stains and environmental wear, which will extend its life span. This is especially critical for applications such as in furniture and automotive upholstery. Towards this, studies are being conducted to optimize the molecular weight of acrylic resin to ensure the comfortness of leather.

## References

[1] Yazdanshenas, M.E., Shateri-Khalilabad, M., 2013. One-step synthesis of superhydrophobicoating on cotton fabric by ultrasound irradiation. Ind. Eng. Chem.Res. 52, 12846e12854
[2] Si, Y., Zhu, H., Chen, L., Jiang, T., Guo, Z., 2015. A multifunctional transparent superhydrophobic gel nanocoating with self-healing properties. Chem. Commun. 51, 16794e16797

# Synthesis of Hydrogen Bonded Copper(II) Coordination Polymer: Photocatalytic Degradation of Rose Bengal Dye and Luminescent Sensing of Hg+2, Cr2O72–, and Nitrofurantoin

**ANAT RAM SIDAR[1] , KAFEEL AHMAD SIDDIQUI[1]***

[1] Department of Chemistry, National Institute of Technology, Raipur, C.G. 492010, India
*Corresponding author: e-mail: vshukla.phd2022.chy@nitrr.ac.in

**Keywords:** Metal Organic Framework, Detection of Anion, Dye Degradation.

A new helical coordination polymer, [Cu(Or)(H2O)3]n has been synthesized at room temperature and examined using single-crystal X-ray diffraction (SC-XRD) and other analytical techniques. [Cu(Or)(H2O)3]n formed 1D helical type structure via coordination bonding as well as a 3D supramolecular network through hydrogen bonding interactions. [Cu(Or)(H2O)3]n manifested as a remarkable luminescent sensor for volatile organic compounds (VOCs), 3-Nitrophenol, Cr2O7 2–, Hg2+ , creatinine, nitrofurantoin and sucrose (200 mg/dl) in particular along with the remarkable photocatalytic degradation of Rose Bengal (RB) dye with 96.54% efficiency. Overall this study demonstrates that the synthesized Cu-orotate coordination polymer has good luminescent sensing and catalytic degradation activity, therefore could be employed for a range of applications such as sensing of biomolecules like sucrose and photocatalysis of toxic dyes.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Micro-textured ETFE for self-cleaning application

Jaishree*, Anupam Bhandari, M.S. Goyat

Department of Applied Science, School of Engineering, University of Petroleum
and Energy Studies,
Dehradun-248007, India
* *Corresponding author e-mail*: jaishreesharma221@gmail.com

**Keywords**: Ethylene tetrafluoroethylene (ETFE); Self-cleaning surfaces; Single-point diamond turning machining

Self-cleaning surfaces have gained considerable attention in the past few years, due to their exceptional applications. Over the past few years, researchers have been claiming ethylene tetrafluoroethylene (ETFE) is a self-cleaning material that can be used to cover solar panels, instead of glass coverings. However, in practice, bare ETFE does not possess a self-cleaning effect as it has a water contact angle of 96.4°. Therefore, ETFE should be micro-textured to generate a self-cleaning effect. In this study, single-point diamond turning (SPDT) machine was used to create a micro-textured surface on the ETFE to induce the self-cleaning effect. Various analytical techniques, including drop shape analysis (DSA), atomic force microscopy (AFM), field-emission scanning electron microscopy (FESEM), thermal gravimetric analysis (TGA), and differential scanning calorimetry (DSC) were employed to evaluate the resulting surface and wetting characteristics. The micro-textured ETFE surface exhibited a water contact angle of 141.2°, which showed high hydrophobicity. Further, the double texturing of ETFE can boost research in this domain to develop self-cleaning superhydrophobic surfaces. These modified surfaces are suitable for a variety of industrial self-cleaning applications.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Investigating Caesium Immobilization in $BaAl_2Ti_6O_{16}$: Synthesis, Characterization, and Leaching Studies

**BHIMARAO M. PATIL**

Department of Chemistry, The Institute of Science, Dr. Homi Bhabha State University, Mumbai, Maharashtra, India
Email: bmpatilisc77@gmail.com

**Keywords**: thermal analysis, tartarate precursor, caesium, nuclear waste

Herein, we present a detailed investigation into the synthesis, characterization, and leaching behavior of caesium-doped $BaAl_2Ti_6O_{16}$, aiming to assess its potential for nuclear waste immobilization. The synthesis involved doping caesium into the $BaAl_2Ti_6O_{16}$ matrix to immobilize caesium for long-term radioactive waste storage. Comprehensive characterization techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDS), were employed to analyze the structural, morphological, and elemental changes induced by caesium doping. The synthesized caesium-doped $BaAl_2Ti_6O_{16}$ exhibited distinct structural modifications confirmed by XRD analysis, demonstrating successful incorporation of caesium into the lattice. SEM imaging revealed morphological changes, while EDS analysis confirmed the homogeneous distribution of caesium within the $BaAl_2Ti_6O_{16}$ matrix. Leaching studies were conducted under elevated temperature conditions to assess caesium release from the material. These results contribute to understanding $BaAl_2Ti_6O_{16}$ as a potential candidate for caesium immobilization. The comprehensive synthesis and characterization, coupled with in-depth leaching studies, offer valuable information for developing effective strategies for the safe disposal of caesium-containing radioactive waste.

**References**

[1] A. E. Ringwood, S. E. Kesson, N. G. Ware, W. Hibberson, A. Major, Nature, 278 (5701) (1979) 219.
[2] J. Amoroso, J. C. Marra, M. Tang, Ye Lin, F. Chen, D. Su, K. S. Brinkma, J. Nucl. Mater., 454 (1–3) (2014) 12.
[3] B. M. Patil, G. C. Wadhawa, A. C. Chaskar, P. S. Walke, Materials Letters, 333, (2023) 133627.
[4] B. M. Patil, G. C. Wadhawa, A. C. Chaskar, P. S. Walke, J Therm Anal Calorim 148, (2023) 7591.

# Evaluation of thermal properties of phase change materials modified with nanoadditives for solar energy harvesting applications

**KATARZYNA SUCHOROWIEC, PIOTR SZATKOWSKI*, KINGA PIELICHOWSKA**
AGH University of Krakow , Faculty of Materials Science and Ceramics,
Department of Biomaterials and Composites
, al. Adama Mickiewicza 30, 30-059 Kraków, Poland
*Corresponding author: e-mail: pszatko@agh.edu.pl

**Keywords**: thermal analysis, DSC, phase-change materials, solar-thermal conversion

Renewable energy sources have attracted a lot of interest in recent years. Sun is an endless source of energy, however it still represents some drawbacks related to the availability in terms of time space and energy losses in the harvesting process [1]. The main advantage of phase change materials (PCM) is that they can store energy as a latent heat thus they could be implemented in thermal energy storage systems to help convert and store solar energy [2]. The incorporation of nanoadditives into PCM materials could work beneficially in terms of solar energy conversion and thermal conductivity improvement.

The aim of this work is to obtain and compare PCM-nanoadditive composites delivered from the eutectic mixture of fatty alcohols and acids with the addition of nanoadditives in the form of graphene (G), nano-$Fe_3O_4$ and carbon nanotubes (CNT).

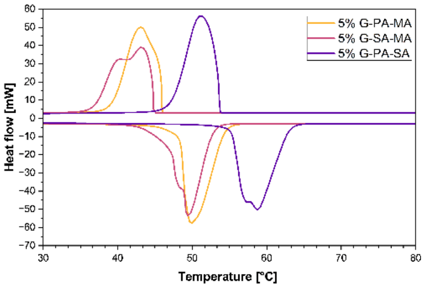


Fig. 1. DSC curves of PCM-Graphene samples

The thermal properties of the composites obtained were analysed using differential scanning calorimetry (DSC) and thermogravimetry (TG). The composite samples were further investigated with scanning electron microscopy (SEM), a leakage test at 80 ° C was performed to establish their shape stability and leakage under increased temperature, and also the performance of the composite under the solar simulator was evaluated. The obtained results reveal that the incorporation of nanoadditives into the eutectic PCM mixtures not only yield the solar-thermal conversion but also could not influence negatively thermal properties of the PCM composites, making them a permissive material for solar energy harvesting and storage.

## Acknowledgments

This work was supported from the subsidy of the Ministry of Education and Science for the AGH University of Science and Technology in Kraków (Project No 16.16.160.557). Research project partly supported by program „Excellence initiative – research university" for the AGH University of Krakow.

**References**

**[1]** B. M. Tripathi, S. K. Shukla and P. K. S. Rathore, *Journal of Energy Storage*, 2023, **72**, 108280.
[2] P. M. Kumar, K. Mylsamy and P. T. Saravanakumar, *Energy Sources, Part A: Recovery, tilization, and Environmental Effects*, 2020,

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Bio-based carbon aerogels infiltrated with sugar alcohols as shape stabilized phase change materials

**MARTYNA SZATKOWSKA[1], KINGA PIELICHOWSKA[1]***

[1]AGH University of Krakow, Faculty of Materials Science and Ceramics, Department of Biomaterials and Composites, al. Mickiewicza 30, 30-059 Kraków, Poland
*Corresponding author: e-mail: kingapie@agh.edu.pl

**Keywords**: thermal analysis, DSC, phase change materials, shape stabilization

Sugar alcohol-based phase-change materials (PCMs) have attracted considerable attention in recent years because of their distinct properties and potential uses in thermal energy storage. Their heat capacity is nearly double that of other organic phase change materials [1,2]. Moreover, due to the ability to cold crystallization can be considered as PCM for long-term thermal energy storage. The main problem with sugar alcohols is their tendency to leak during phase transition processes (solid-liquid transition) [3]. The solution to this problem proposed in literature is shape stabilization by using carbonized materials with a porous structure (watermelon) [4].

The main goal of our research was to obtain a phase change material with shape stabilization for long-term energy storage. For this purpose, carbon aerogels obtained by carbonization of orange peel, pomelo peel and pomelo peel modified with starch (2,5; 5; 10 and 20 wt.%) were obtained. Next, carbon aerogels were infiltrated with sugar alcohol-based PCMs. To characterize properties of the obtained PCM composites differential scanning calorimetry (DSC), modulated temperature DSC (TOPEM), step-mode DSC, thermogravimetric analysis (TGA) and scanning electron microscope (SEM) were used. Additionally, the percentage of PCM infiltrated into the carbonized fruit biomass was calculated.

## Acknowledgments

This work was supported from the subsidy of the Ministry of Education and Science for the AGH University of Science and Technology in Kraków (Project No 16.16.160.557). Research project partly supported by program „Excellence initiative – research university" for the AGH University of Krakow.

## References

[1] R. Jia, et al., The Journal of Chemical Thermodynamics, 2017, 115, 233–248

[2] S. T. Latibari, et al., Solar Energy, 2018, 170, 1130–1161.

[3] K. Pielichowska et al, J. Appl. Polym. Sci., 2010.

[4] H. Liu, et al., ACS Appl. Energy Mater., 2021, 4, 1714–1730.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Enhancing the properties of phase change materials (PCMs) by carbon-based materials for electo-thermal conversion

**PIOTR SZATKOWSKI[1]*, RAFAŁ TWARÓG[2], KINGA PIELICHOWSKA[2,3]**

AGH University of Krakow , Faculty of Materials Science and Ceramics,
Department of Biomaterials and Composites,
al. Adama Mickiewicza 30, 30-059 Kraków, Poland
*Corresponding author: e-mail: pszatko@agh.edu.pl

**Keywords**: thermal analysis, DSC, phase change materials, electro-thermal conversion

Phase change materials (PCMs) have emerged as a promising technology for thermal energy storage (TES) because of their ability to absorb and release large amounts of latent heat during phase transitions. This unique property makes PCMs ideal candidates for a wide range of applications, including thermal regulation in buildings, solar energy storage, and electronic cooling. However, conventional PCMs often suffer from limitations such as low thermal conductivity, high melting/solidification temperatures, and phase separation issues. Phase change materials (PCMs) can store excess electrical energy in the form of latent heat. During the charging process, excess electricity is converted into heat using a resistance heater or heat pump. This heat is then absorbed by the PCM as it melts, storing the energy for later use. Some common PCMs include paraffin waxes, salt hydrates, and metallic alloys. The choice of PCM for a particular application depends on several factors, such as the desired operating temperature range, energy density, and cycle life.  The main goal of this research was to obtain a phase change material with shape stabilisation with porous carbon materials and modified with carbon nanomaterials for electrothermal conversion. For this purpose, porous carbon materials were obtained by carbonization of waste biomass. Next, porous carbon materials were infiltrated with selected PCMs modified with carbon nanoadditives. To characterize properties of the obtained PCM systems differential scanning calorimetry (DSC), modulated temperature DSC (TOPEM) and step-mode DSC were applied. Therma stability was assessed using thermogravimetric analysis (TGA).

**Acknowledgments**

This work was supported from the subsidy of the Ministry of Education and Science for the AGH University of Science and Technology in Kraków (Project No 16.16.160.557). Research project partly supported by program „Excellence initiative – research university" for the AGH University of Krakow.

**References**

[1] Kulish, V., Aslfattahi, N., Schmirler, M. et al. New library of phase-change materials with their selection by the Rényi entropy method. Sci Rep **13**, 10446 (2023).

# Molecular Dynamics Simulations Study on Structural and Thermodynamic Analysis of Mixtures of Oxidized and Unoxidized Forms of Polyaniline

**CHAITANYA DHARMENDRAKUMAR GANDHI*; PRAVEENKUMAR SAPPIDI**

Department of Chemical Engineering, Indian Institute of Technology Jodhpur 342037, India
Department of Chemical Engineering, Indian Institute of Technology Jodhpur 342037, India
*Corresponding author: e-mail: gandhi.4@iitj.ac.in

**Keywords:** MD simulations, Polyaniline, Umbrella sampling, Structural properties, Conductive membrane

Conducting polymers such as polyaniline (PANI) has shown a significant interest in the field of electrified membranes (EMs) with antifouling properties. EMs utilize charged or conductive polymers to prepare the membrane surface. These membranes may form electroactivity to mitigate fouling.[1] However, blending/doping of PANI with other polymers and nanomaterials highly influences the properties of the membrane surface.[2] PANI has both oxidized and unoxidized forms namely, emeraldine salt (ES) and emeraldine base (EB), respectively. Therefore, understanding the PANI structure with the variation of the oxidized and unoxidized forms along the length of the polymer chain is Intriguing. In this work, we present the design of the novel copolymer consisting of EB and ES monomers with varying charge densities and arrangements (Figure 1).

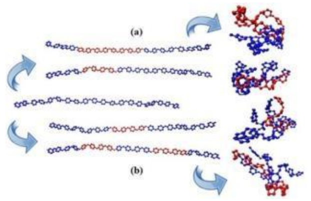


Fig. 1: Arrangements of the monomers in the polymeric chain with umbrella sampling (a) random and (b) sequential. Color code: Blue- EB and red-ES.

We present various intra and intermolecular structural properties of the PANI chain. Our results show increased radius of gyration ($R_g$) values with the increase in charge density. Furthermore, we also present a detailed conformational free energy analysis to understand the PANI chain conformational transition.[4] H-bonding, SDFs, and SASA values lead to uncoiling and increased conductivity of the chain. These observations are crucial in understanding the complex behavior of the chains for the design of anti-fouling electrified membranes.

## References

(1) Li, N.; Lou, T.-J.; Wang, W.; Li, M.; Jing, L.-C.; Yang, Z.-X.; Chang, R.-Y.; Li, J.; Geng, H.-Z. *J Memb Sci*, 668 (**2023)** 121271.
(2) Wang, K.; Xu, L.; Li, K.; Liu, L.; Zhang, Y.; Wang, *J. J Memb Sci*, (**2019**) 570–571, 371–379.
(3) Dharmendrakumar Gandhi, C.; Sappidi, *P. J Mol Liq*, 402(**2024**) 124748.
(4) Lemkul, J. A.; Bevan, *D. R. J Phys Chem B.*, 114(4) (**2010**) 1652–1660.

# Synthesis and Characterization of Biobased multiblock copolymers: Poly(ethylene2,5-furandicarboxylate)- b -Poly(ε-caprolactone) targeting food packaging applications.

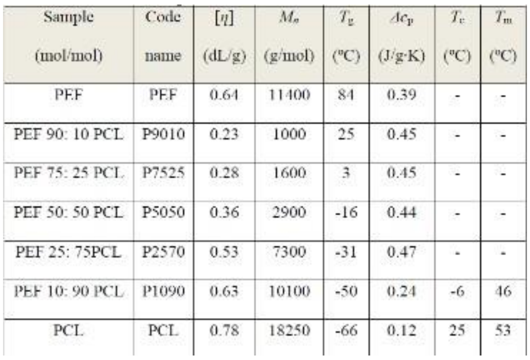
**JOHAN STANLEY[1*], DIMITRA A. LAMBROPOULOU [2,3], DIMITRIOS N. BIKIARIS[1]**

[1]Laboratory of Chemistry and Technology of Polymers and Colors, Department of Chemistry,
Aristotle University of Thessaloniki, Thessaloniki, Greece.
[2]Laboratory of Environmental Pollution Control, Department of Chemistry,
Aristotle University of Thessaloniki, GR–541 24 Thessaloniki, Greece.
[3]Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Balkan Center,
GR-570 01 Thessaloniki, Greece.
*Corresponding author: e-mail: ohansta@chem.auth.gr

**Keywords**: Poly(ethylene 2,5-furan dicarboxylate), Poly(ε-caprolactone), biobased polyester, Thermal properties.

Poly(ethylene 2,5-furan dicarboxylate) (PEF) is a 100% biobased polymer with superior thermal (higher glass transition temperature and lower melting point) and barrier properties (oxygen, carbon dioxide, and water barrier) compared to poly(ethylene terephthalate) (PET). [1] In present work, A series of multiblock copolymers poly(ethylene 2,5-furandicarboxylate)- Poly(ε-caprolactone) (PCL) were synthesized through a two-step melt polycondensation method targeting food packaging applications as displayed in Table 1.

Table 1: Samples list and main calorimetric values



| Sample (mol/mol) | Code name | $[\eta]$ (dL/g) | $M_n$ (g/mol) | $T_g$ (°C) | $\Delta c_p$ (J/g·K) | $T_c$ (°C) | $T_m$ (°C) |
|---|---|---|---|---|---|---|---|
| PEF | PEF | 0.64 | 11400 | 84 | 0.39 | - | - |
| PEF 90: 10 PCL | P9010 | 0.23 | 1000 | 25 | 0.45 | - | - |
| PEF 75: 25 PCL | P7525 | 0.28 | 1600 | 3 | 0.45 | - | - |
| PEF 50: 50 PCL | P5050 | 0.36 | 2900 | -16 | 0.44 | - | - |
| PEF 25: 75PCL | P2570 | 0.53 | 7300 | -31 | 0.47 | - | - |
| PEF 10: 90 PCL | P1090 | 0.63 | 10100 | -50 | 0.24 | -6 | 46 |
| PCL | PCL | 0.78 | 18250 | -66 | 0.12 | 25 | 53 |

Attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR) results showed PCL was successfully introduced into the polymer chain. [2] Differential scanning calorimetry (DSC) results demonstrated that single glass transition steps and mainly vanishing of the PCL's crystallizability, that are almost direct evidence of the excellent PCL/PEF distribution, without neither micrometric nor nanometric phase separation. A significant plasticizing role of PCL over PEF, as manifested by the systematic drop in Tg.

## References

[1] J. Louw, S. Farzad, J.F. Görgens, Polyethylene furanoate: technoeconomic analysis of biobased production, Biofuels, Bioproducts and Biorefining 17 (2023), pp. 135–152

[2] J. Wang, X. Liu, Z. Jia, Y. Liu, L. Sun, J. Zhu, Synthesis of bio-based poly (ethylene 2, 5-furandicarboxylate) copolyesters: Higher glass transition temperature, better transparency, and good barrier properties. J. Polym. Sci. A Polym. Chem. 55 (19), (2017), pp. 3298– 3307.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Thermal Behavior of Low Density Polyethylene for Agricultural Applications

**I. BLANCO[1]*, G. RIZZO[1], V. SIRACUSA[2]**

[1] Department of Civil Engineering and Architecture, University of Catania, Via Santa Sofia 64, Catania, 95125, Italy
[2] Department of Chemistry, University of Catania, Via Santa Sofia 64, Catania, 95125, Italy
*Corresponding author: iblanco@unict.it

**Keywords**: thermogravimetric analysis, DSC, polymers, agricultural

Polyethylene (PE) is durable, and has low stiffness, but has high toughness and impact resistance as well as low friction. Low-density polyethylene (LDPE) has more branches (about 2% of carbon atoms) than high-density polyethylene (HDPE), so its intermolecular forces (bipolar-bipolar attraction) are weak, its tension is lower, and its resistance is higher. Thus, since its molecules are not tightly packed and less crystalline due to lateral branches, its density is lower.

LDPE is suitable for thermoplastic mold processing and good mold making capabilities, its main uses are in packaging (bags, films, seismic screens, bottles, etc.) [1,2]. In the last twenty years, the wide distribution of protected cultivation has increased the production and marketing of a large variety of greenhouse covering materials, among LDPE films plays a dominant role in the sector [3].

In this study, LDPE films for agricultural applications were sprayed with pesticides and their thermomechanical performance was evaluated, compared to uncontaminated samples, through techniques such as thermogravimetry, differential scanning calorimetry and dynamic mechanical analysis.

It was observed how the pesticide treatment affected the thermal properties, such as the glass transition temperature, the melting temperature and the initial decomposition temperature.

**References**

[1] D. Duraccio, C. Silvestre, M. Pezzuto, S. Cimmino, A. Marra, in: C. Silvestre, S. Cimmino (Eds.). *Ecosustainable Polymer Nanomaterials for Food Packaging*, CRC Press, London, 2013
[2] I. Blanco, *Journal of Thermal Analysis and Calorimetry* 125 **(2016)** 809.
[3] D. Briassoulis, *Polymer Degradation and Stability*, 88 **(2005)** 489.

# Zwitterion-modified chitosan derivatives for dental applications: Synthesis and thermal properties characterization

**DIMITRIOS N. BIKIARIS**[1]*, **EVI CHRISTODOULOU**[1], **GEORGIA MICHAILIDOU**[1], **ELEANA KONTONASAKI**[2]

[1] Laboratory of Polymer and Colors Chemistry and Technology, Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece

[2] Department of Prosthodontics, School of Dentistry, Faculty of Health Sciences, Aristotle University of Thessaloniki, Thessaloniki, Greece.

*Corresponding author: e-mail: dbic@chem.auth.gr

**Keywords**: chitosan modification, zwitterions, spectroscopy, XRD, TGA

Chitosan (CS) is a natural polysaccharide vastly applied in pharmaceutical and biomedical applications, due to its favourable characteristics, including its biocompatibility and biodegradability, the enhanced antioxidant and innate antibacterial properties, and its non-toxicity. Zwitterions are molecules that contain positively and negatively charged groups, resulting in an overall neutral charge. They are able to reduce non-specific protein adsorption, as well as bacterial adhesion, and thus provide an improved antibacterial behaviour and increased bioavailability when used in the delivery active compounds.

For this purpose, in the present work, three zwitterion-modified CS derivatives (using monomers 2-(methacryloyloxy)ethyl]dimethyl-(3-sulfopropyl) ammonium (SBMA), 2-acrylamido-2-methyl-1-propanesulfonic acid (AMPS), and 2-sulfobenzoic acid cyclic anhydride (SBA)) in two different molar ratios (4/1 and 10/1) were prepared and comparatively studied. The successful modification of CS structure was confirmed spectroscopically using FTIR and $^1$H-NMR, and the molecular weight in relation to the viscosity properties of the prepared derivatives was studied. The crystalline structure was assessed via XRD, indicating a drop in the degree of crystallinity compared to neat CS in all cases, due to the insertion of the zwitterionic monomers that interrupts the macromolecular chain folding and the subsequent crystallite formation. TGA curves were also recorded (Fig 1) in order to examine the effect of modification on thermal stability, showing a two-stage degradation procedure.

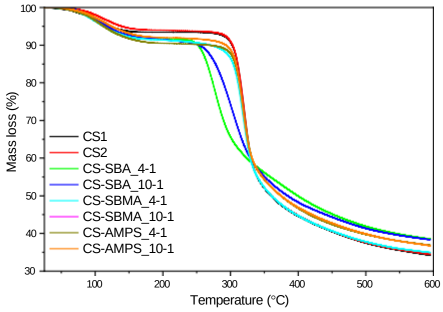


Fig. 1: TGA thermograms of neat CS and the prepared CS derivatives.

**Acknowledgments:** The project I-SMarD has received funding from the European Union's Horizon 2020 Research and Innovation Program under Grant Agreement No 953128.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Unravelling the Stabilization Mechanism of Mono-, Di, and TriCholinium Citrate-Ethylene Glycol DESs towards α-Chymotrypsin for Preservation and Activation of the Enzyme.

**BINDU YADAV[1], NIKETA YADAV[2], PANNURU VENKATESU***

[1,2],* Department Of Chemistry, University Of Delhi,110007, India
*Corresponding author: e-mail: venkatesup@hotmail.com

**Key Words:** Deep eutectic solvents, Biocompatibility, Proteolytic activity, Structural stability

In view of global challenges posed by conventional organic solvents, Deep Eutectic Solvents (DESs) have emerged as a more environmentally friendly option, particularly for enzymes. However, there is a lack of understanding regarding how various multicationic DES systems affect biomolecules. To address this, we synthesized three DESs- monocholinium citrate-ethylene glycol ([Chn][Cit] -EG), dicholinium citrate-ethylene glycol ([Chn]2[Cit]-EG), and tricholinium citrate ethylene glycol ([Chn]3[Cit]-EG) and examined their suitability for α-chymotrypsin (α-CT). Specifically, we investigated how increasing the cationic ratio of the hydrogen bond donor (HBA) affects the stability and activity of α-CT using spectroscopic techniques. Our analyses revealed enhanced structural stability and activity of α-CT with increasing cationic ratio of DESs. Interestingly, we observed better structural stability of α-CT in ([Chn]3[Cit]-EG) and ([Chn]2[Cit]-EG) compared to ([Chn]3[Cit]-EG). Notably, temperature-dependent fluorescence spectroscopy showed that the transition temperature (Tm) of α-CT increased in the presence of all three DESs compared to the buffer solution, highest in ([Chn]2[Cit]-EG). These findings demonstrate that increasing the molar ratio of aqueous cholinium cation in [Chn][Cit] enhances DESs ability to stabilize α-CT. Altogether, this study offers new perspectives on how the stability and structural changes of proteins depend on the composition of Deep Eutectic Solvents (DESs). It also demonstrates how modifying the molar ratios HBA of DES components can adjust the biocompatibility of DESs with enzymes, thus expanding their potential applications in biocatalysis

## References

[1] Yadav, N.; Bhakuni, K.; Bisht, M.; Bahadur, I.; Venkatesu, P. ACS Sustain. Chem. Eng. 2020, 8(27), 10151–10160.
[2] Kumar, A.; Venkatesu, P. Chem. Rev. 2012, 112 (7), 4283–4307.
[3] Sindhu, A.; Bisht, M.; Bahadur, I.; Venkatesu, P. ACS Sustain. Chem. Eng. 2021, 9 (13), 4812– 4822

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Impact of imidazolium type Zwitter Ion Ionic Liquids on peroxidase activity and conformational stability of cytochrome c

**POOJA YADAV[1], PANNURU VENKATESU[*]**
[1, *] Department of Chemistry, University of Delhi,110007, India
*Corresponding author: e-mail: venkatesup@hotmail.com

**Keywords**: Zwitter ions, Cytochrome c, imidazolium based ionic liquids

There is considerable interest in the use of structurally stable and catalytically active enzymes, such as cytochrome c (Cyt c), in the pharmaceutical and fine chemicals industries. However, harsh process conditions, such as temperature, pH, and the presence of organic solvents, are the major barrier to the effective use of enzymes in biocatalysis. Functional Zwitter Ions (ZIs) developed from Ionic Liquids (ILs) are anticipated to exhibit IL-like characteristics because the word "zwitterion" itself indicates an ion pair where the cation and anion are covalently linked. There are some particular characteristics that ZIILs alone can display like cytochrome c gets renatured dissolved in polar phosphonate type ionic liquids by using highly polar ZIs, Phosphonate type zwitter ion used as an additive to improve the saturated water content of phase separated ionic liquid from aqueous phase towards reversible extraction of proteins. We demonstrate the suitability of imidazolium-based ZIILs as potential media for enzymes, in which remarkable enhanced activity and improved stability of Cyt c against multiple stresses were obtained. Among the several ZIILs studied, we observed the increase conformational stability and activity of Cyt c in the aqueous solutions of 4-(3-methyl-1H-imidazol-3-ium-1-yl) butane-1-sulfonate, 4-(3-ethyl-1Himidazol-3-ium-1-yl) butane-1-sulfonate, 4-(3-butyl-1H-imidazol-3-ium-1-yl) butane-1-sulfonate and 4- (3-hexyl-1H-imidazol-3-ium-1-yl) butane-1-sulfonate compared to the commonly used phosphate buffer solutions (pH 7.2). The observed enzyme activity is in agreement with its structural stability, as confirmed by UV–vis, circular dichroism (CD). Moreover, it was found that the imidazolium-based ILs studied herein protect the enzyme against protease digestion and allow long-term storage at room temperature monitored by UV-vis spectroscopy and activity.

**References**

[1] Bisht, M.; Mondal, D.; Pereira, M. M.; Freire, M. G.; Venkatesu, P.; Coutinho, J. A. P. Long-Term Protein Packaging in CholiniumBased Ionic Liquids: Improved Catalytic Activity and Enhanced Stability of Cytochrome C against Multiple Stresses. Green Chem. 2017, 19, 4900−4911.

[2] Lozano, P.; De Diego, T.; Gmouh, S.; Vaultier, M.; Iborra, J. L. Dynamic structure-function relationships in enzyme stabilization by ionic liquids. Biocatal. Biotransform. 2005, 23, 169−176

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Enhanced Thermoresponsive Behaviour in MXene-Embedded PVCL Composites: Lowered LCST and Potential Biomedical Applications

**POOJA[1], P. VENKATESU***

Department of Chemistry, University of Delhi, Delhi-110007, India
*Corresponding author: e-mail: venkatesup@hotmail.com

**Keywords**: Polymer composites, MXenes, DLS, LCST

The advancement of smart polymers is pivotal in the evolution of drug delivery systems. The alteration in characteristic properties of the polymer in response to physiological stimuli has emerged as a promising strategy. Herein, we report a significant step forward by studying the effect of MXenes in particular $Ti_3C_2$ single layered (SL), $Ti_3C_2$ stack, and $V_2C$ stack on the LCST of polymer; PVCL in aqueous solution. An array of biophysical techniques such as UV-visible spectroscopy, Steady-state fluorescence spectroscopy, DLS, Zeta potential measurement, and FTIR were employed to probe into the intricate dynamics of phase transitions of PVCL. For assessing topography and surface morphology AFM, TEM, and FESEM were utilized. Our findings reveal a discernible reduction in LCST in the presence of all three MXenes, attributed primarily to the creation of a more hydrophobic microenvironment facilitated by MXenes. MXenes effectively modulate the interaction of PVCL with water molecules, leading to destabilization of the hydrated macromolecular structure and subsequent premature hydrophobic collapse of PVCL. Importantly, LCST was found to be tunable upon the incorporation of MXenes, with an observed shift of 3ºC and 2ºC for $Ti_3C_2$ (SL), $Ti_3C_2$ stack , and $V_2C$ stack respectively. This study is of immense importance as the conjugates formed can be harnessed to design smart drug delivery systems.

**References**

[1] Ritu Yadav, Krishan Kumar, Sumit Kumar, Sanjay Mor, and Pannuru Venkatesu, *Langmuir* **2023**, *39* (13), 4809-4818.
[2] A Rajbanshi, E Hilton, CA Dreiss, D Murnane, MT Cook, *Macromolecular Rapid Communications*, **2024,** 2300723.
[3] I Rad, E Esmaeili, BB Jahromi, *Polymer Bulletin*, **2024**,1-22.

# Study of Novel Surfactant Based Spectroscopically Active Ionic Liquids

**PRATAP K. CHHOTARAY[1]*, MOLOY SARKAR[2]**

[1]Department of Chemistry, Centurion University of Technology and Management, Bhubaneswar, 752050, India
[2]Department of Chemistry, National Institute of Science Education and Research, Bhubaneswar, 752050, India
*Corresponding author: e-mail: pratap.chhotaray@cutm.ac.in

**Keywords**: Ionic liquids, Surfactant, Dye, Fluorescence.

Restricted solubility of dyes' limited the biomedical imaging applications. Similarly, the drug internalization mechanism for surfactants has not been understood completely. Both of their limitations can be resolved by combining them into a single entity.

Eosin Y sodium salt (EoY) was combined with Cetylpyridinium chloride monohydrate (CePy) in a 1:1 molar ratio to get Surfactant Based Spectroscopically Active Ionic Liquid (SAIL). The $^1$H NMR and ATR-FTIR spectrum of synthesized SAIL clearly shows the peak shift when compared to starting materials which signifies the formation of new compounds.

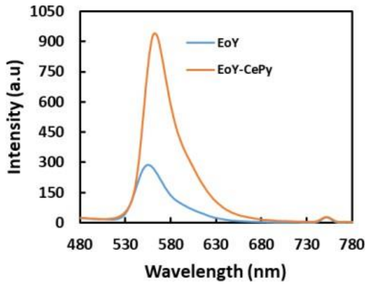


Fig. 1: Fluorescence spectrum of EoY dye and EoY-CePy SAIL.

The UV-visible investigation also shows a 4 nm shift of $\lambda_{max}$ towards a longer wavelength from the dye (EoY) to SAIL. A shift in fluorescence peak as depicted in Figure 1, was observed from 554 nm to 562 nm for dye and SAIL, respectively. This shift in peak also suggests the formation of SAIL. Further investigations such as mass spectrometry, TGA, DSC, etc. will be carried out to understand macroscopic behavior. The synthesized SAILs would be helpful for biomedical applications such as deep tissue imaging and drug solubility.

**References**
[1] B. Gohain, S. Sarma, R. K. Dutta, *J. Mol. Liq.*, 142 (**2008**) 130.
[2] S. Gokturk, M. Tuncay, *J. Surf. Det.*, 6 (**2003**) 325.
[3] K. M. Sachin, S. A. Karpe, M. Singh, A. Bhattarai, *Heliyon*, 5. **(2019)**, 210.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Nanoparticle assisted micro gelation enhanced carbon capture through modified amines using absorption from simulated flue gas stream

**YOGENDRA KUMAR, JITENDRA SANGWAI***

Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai-600036, India
*Corresponding author: e-mail: ch21d005@smail.iitm.ac.in,
jitendrasangwai@iitm.ac.in

**Keywords**: amine, absorption, carbon capture, DEA, flue gas, thermal analysis.

## Abstract

Capturing $CO_2$ directly from human-generated emissions is a crucial societal obligation, given the concerning increase in global atmospheric $CO_2$ levels. Achieving net zero and making industrial clusters carbon neutral is challenging and not possible without developing large scale carbon capture technology directly from industrial flue gases. While amine-based absorbents have traditionally been used for carbon capture, their effectiveness is limited due to issues such as high temperature requirements, energy-intensive regeneration, poor recyclability, and corrosion problems. This study introduces a nanoformulation derived from amines to demonstrate a sustainable $CO_2$ absorption process, aiming to improve carbon capture performance and lower regeneration costs for large-scale industrial applications. Experiments were conducted in interfacial contact batch reactor at 298 and 318 K temperature using $N_2$+$CO_2$ mixture with nanoformulation and conventional DEA amine solutions. The nanoformulation, prepared using microgelated nanoparticles, additives and conventional amines through a three-step preparation technique, showcases a notable enhancement in capture efficiency, approximately 30% higher than conventional amine solvents. Additionally, it exhibits superior recyclability, retaining effectiveness for up to five cycles in an interfacial contact reactor system. Furthermore, the nanoformulation displays the ability to absorb $CO_2$ at faster rates compared to traditional DEA solutions. When combined with other contacting strategies, this approach holds promising prospects for carbon capture at industrial scales or directly from the air.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Eco-Conscious Innovation: Creating a Sustainable Biodegradable Polymer from Citrus Peels and Investigating its Soil Microbial Degradation

**S. RAMANAIAH**[*1], **S.VEENA**[2], **M. E. RANI**[2]

[*1]Dept. of Chemistry, Sri Venkateswara College, University of Delhi, New Delhi-110021, India

[2]Department of Chemistry, Rayalaseema University, Kurnool, Andhra Pradesh - 518007, India

*Corresponding author: e-mail: sramanaiah@svc.ac.in

**Keywords**: bioplastics, orange peels, microorganisms in soil, biodegradable

The aim of the present research investigation is to synthesis the bioplastic from naturally available source of fruit waste. Unlike conventional plastics made from fossil fuels, these are bio-based and can be fully or partially biodegradable. The development of bioplastics is the solution of the new era to control the adverse impact of conventional plastics on the environment. Plastics that are biodegradable and made from natural materials should be considered as an immediate alternative to them. They provide companies with environmentally friendly alternatives for packaging and products, especially for disposable items that generate a lot of waste. The bioplastics industry is still in its infant but is growing steadily and will gradually replace many disposable items made from petroleum-based plastic, such as cups, cutlery, packaging, containers and straws. However, these cannot compete with traditional plastics in terms of cost and performance. Therefore, to increase the performance of bio-based polymers, orange peels, a fruit waste, are used as raw material because they are rich in cellulose. Simple laboratory techniques are used to synthesize a biopolymer. The synthesized biopolymer film is blended with a plasticizer such as glycerol, and promising results have been observed in terms of tensile strength and flexibility. X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy characterization confirmed that the polymer film synthesized from orange peel is a bio-based plastic. Degradation studies were performed for the synthesized film in soil, the interaction between bioplastics and soil microbes were clearly investigated. This process of degradation by microorganisms affects the nitrogen cycle in the soil. In addition, the rate of degradation depends on the main components used in the synthesis of bioplastics. The results showed that the bioplastic produced from orange peel is biodegradable, decomposes in the environment, and can also be used as an alternative source for conventional plastics.

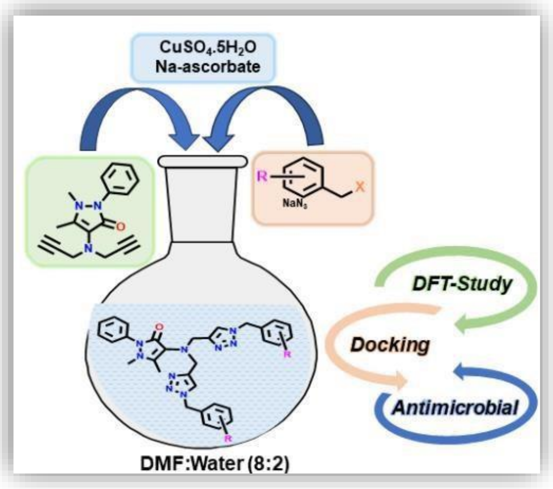
# Design, Synthesis, and Studies (Antimicrobial Activity, Molecular Docking, and DFT) of Ampyrone linked Bis-triazoles

**Bajrang Lal, Ram Kumar Tittal***

Department of Chemistry, National Institute of Technology Kurukshetra, Haryana-136119, India.
*Corresponding author: e-mail: rktittaliitd@nitkkr.ac.in

**Keywords:** Ampyrone, Bis-1,2,3-triazole, Anti-microbial activity, Molecular docking, and DFT study.

A new class of bis-triazoles linked with ampyrone molecules was synthesized from ampyrone-linked bis-alkyne with different benzyl azides under Cu(I)-catalyzed azide-alkyne cycloaddition (CuAAC) reaction. All compounds were characterized by FTIR, $^{1}$H-NMR, $^{13}$C-NMR, and ESI-MS data. However, the structures of solid crystalline compounds **4a** and **4h** were finally supported by X-ray crystallographic data. *In vitro*, anti-microbial activity results of synthesized alkyne **2** and bis-1,2,3-triazoles **4a-4k** showed that incorporation of triazole units has augmented the anti-microbial activity of all compounds, except **4a** for *E. coli*. Also, compound **4f** was found potent against all bacterial strains (*E. coli*, *S. aureus*, and *P. aeruginosa* each with MIC: 0.0178 µmol/mL) with superior efficacy to *B. subtilis* (MIC: 0.0089 µmol/mL) compared to standard antibacterial drug ciprofloxacin (MIC: 0.0094 µmol/m). Almost all synthesized triazoles showed superior potency to both fungal strains except **4a**, **4g**, and **4k** against *R. oryaze*, *C. albicans*, and *R. oryaze*, respectively. Computational molecular docking and DFT results also supported experimental anti-microbial results for improvement in the activity of all triazoles except, **4a**.



**References**

[1] K. Bozorov, J. Zhao, and H.A. Aisa, *Bioorganic Medicinal Chem*istry 27 (2019) 3511–3531.
[2] N. Nehra, R.K. Tittal, and D. Ghule Vikas, *Jouranl of Molecualr Structure* 1245 (2021) 131013.

**T7- PP 02**

# Computational and Thermodynamic Analyses for Rapid Drug Repurposing: Insights into Viral Pandemics and Therapeutic Candidates

***SK. MD NAYEEMA, SK. MD RAMEEZ ARHANB, SK. SHIREENC, D, M. SRINIVASA REDDYE**

[*a] Department of Physics, KRK Government Degree College, Addanki-523201, AP., India
[b]Department of Mechanical Engineering, National Institute of Technology, Warangal-506004, TS, India.
[c]Capgemini Technology Services India Limited, Financial District, Kokapet, Hyderabad-500006, TS, India.
[d]Department of Data Science & Applications (MPS), State University of New York-University at Buffalo, Buffalo- 14260, USA
[e]Department of Chemistry, DS(W) Government Degree College, Ongole-523001, AP., India.

*Corresponding author: shaikmahammadnayeem2@gmail.com

**Keywords**: Computational Drug Repurposing, Molecular Dynamics Simulation, Thermodynamic Analysis, Viral Pandemics, Monkeypox, Drug-Protein Interactions, Therapeutic Candidates

This study employs computational methodologies, specifically molecular dynamics simulations and thermodynamic analyses, to explore the feasibility of rapid drug repurposing during viral pandemics, exemplified by Monkeypox. We focus on assessing drug-protein interactions at the atomic level, aiming to expedite the identification of potential therapeutic candidates. Our findings support and extend the assertions made in the abstract. Notably, our results reveal robust binding interactions of Tecovirimat, with greater flexibility compared to Brincidofovir, with the Monkeypox virus, which may be advantageous in evolving contexts. The computational study aligns with universal medical trials. These outcomes, while preliminary, offer valuable insights into potential therapeutic avenues, emphasizing the crucial role of computational approaches in pandemic response strategies.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Synthesis and Antifungal Activity of Some Coumarin-based 1,2,3-Triazole Derivatives: A Review.

**NANDINI DAVE[1], PRAKASH CHANDRA[2], MANOJ PANDEY[1]***

[1,2]Department of Chemistry, Pandit Deendayal Energy University, Gandhinagar, Gujarat – 382426
*Corresponding author: e-mail: manoj.pandey@sot.pdpu.ac.in

**Keywords:** 1,2,3-triazole, Antifungal activity, Click Chemistry approach

Using a click chemistry technique, novel coumarin-based 1,2,3-triazole derivatives were synthesized from 4-hydroxy coumarin and several substituted azides in an attempt to create a "hybrid molecule with linker" that would be physiologically active. N-(substituted phenyl)2-(4-(((2-oxo-2H-chromen-4-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)acetamide] is a kind of triazole chemical that was synthesized by reacting copper sulphate with sodium ascorbate and a combination of solvents as a catalyst. Compounds were thoroughly characterized by the application of several spectroscopic methods. Using the agar cup-plate technique, synthesized triazole compounds were evaluated for their antifungal activity against a variety of fungal species.

## References

[1] E. Clarke, Jarvis CI, Goncalves MB, Kalindjian SB, Adams DR, Brown JT, Shiers JJ, Taddei DMA, Ravier E, Barlow S, Miller I, Smith V, Borthwick AD, Corcoran JPT, Bioorganic & Medicinal Chemistry 26(4) (2018)798–814.
[2] Meunier B (2008) Hybrid Molecules with a Dual Mode of Action: Dream or Reality? Acc Chem Res 41(1):69–77.
[3] Z. Rezaei, S. Khabnadideh, K. Pakshir, Z. Hossaini, F. Amiri, E. Assadpour, European Journal of Medicinal Chemistry 44(7) (2009) 3064–3067

18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024

# Automation in process safety information delivery

**[1]Syed Tanweer Ahmed*, [2]Han Xia**

[1]Advisor-II, [2]Senior Advisor
Chemical hazard lab, Eli Lilly and Company, Bengaluru, India, 560102
*Corresponding author: e-mail: syed_tanweer_a@lilly.com

In pharmaceutical industry we often work with new molecules and intermediate whose thermal information is unknown. The general lack of information relevant to the thermal/reactive hazards associated with the use of chemicals sometimes result in incidents or near misses when we failed to recognize the potential hazards. Therefore, thermal hazards associated with chemicals in use need to be known. Then the questions come*; How safe are the materials that we are using? Can we ship and store them? Is it safe to use the material in process?* In these circumstances automation of process safety information delivery can be a helping hand.

Here we propose a desktop screening method based on energy density of molecule to early identify and deliver safety information to chemist/engineer. It identifies number of high energy functional group in a molecule (*Based on United Nation list*) and calculates energy density. A web interface has been developed to facilitate easy access to information, furthermore the web interface can fetch information related to molecules such as, internal DSC data, Yoshida explosivity information, Bretherick's handbook data, etc. Combinedly, the web interface makes process safety information package, and it only requires molecular structure as input and scale of reaction.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Repurposing Fluoroquinolone Drugs for the Treatment of Actinopathy-Induced Neurodegeneration

**RAHUL GUPTA[1], AVINASH KALE[1]***

[1]School of Chemical Sciences, UM-DAE Center for excellence in basic sciences, University of Mumbai 400098, Maharashtra, India.
*Corresponding author: e-mail: avinash.kale@cbs.ac.in

**Keywords**: fluoroquinolones, DSC, actin, biophysical studies, neurodegeneration

In recent years, Alzheimer's and Parkinson's research has focused on AB plaques and tau protein[1]. However, understanding of actin-associated actinopathic structures such as Hirano bodies is limited. Finding novel therapeutic candidates is laborious and expensive process therefore exploring alternative functions of FDA-approved molecules for age-related actinopathies is essential[2]. In the current study, we explored the effect of fluoroquinolones on actin depolymerization dynamics using a variety of biophysical techniques. We have found using light scattering studies, the drugs induce actin disaggregation, and the same was confirmed using size exclusion chromatography. The protein aggregates remain heterogeneous even at elevated drug concentrations with minor adaptive secondary structural changes. Using DSC, reduction in protein melting temperature and calorimetric ΔH with increasing drug concentration indicates drug induced destabilization of filamentous protein structure. The observation is in agreement with our in vitro assays and in-vivo actin disaggregation assay in *Saccharomyces cerevisiae* Δend3 mutant cells[3]. We have also conducted in-silico docking studies to deduce plausible mechanism of drug binding to the actin protein as well as for identification of binding sites and clusters.

Based on the findings, we infer that fluoroquinolones when attached to a proper drug delivery system, can be good potential candidates for the treatment of actinopathic neurodegenerative disorders.

**References**

[1] J.R.Bamburg, B.W Bernstein, 73(9) (**2016)** 477–97.

[2] W.Spears, M. Furgerson, J.M. Sweetnam, P.Evans, M.Gearing, M. Fechheimer, et al. *BMC Neurosci.* 15 (**2014**) 1–20.

[3] H. Benedetti, S. Raths, F.Crausaz, H.Riezman, *Biol Cell.*, 84(1-2) (**1995**) 119–119.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Extraction of DNA using Ionic Liquid-based Aqueous Biphasic System

**K. K. ATHIRA*, J. MEPPERI, H. C. KOTAMARTHI, R. L. GARDAS**

Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036, India
*Corresponding author: e-mail: gardas@iitm.ac.in

**Keywords**: solvent extraction, plasmid DNA, anion optimization

The separation and purification of nucleic acid is a widely studied field as it has paramount importance. The disadvantages of conventional extraction methods include toxicity, complexity and time consumption [1]. The search for an alternative method for DNA extraction studies has led to ionic liquid (IL) based aqueous biphasic systems which is a benign method for biomolecule extraction [2]. The present work is focused on developing an ABS constituting ammonium-based ionic liquids (ILs) and phosphate buffer ($K_2HPO_4$-$KH_2PO_4$) for the partitioning of DNA. Additionally, the stability of the DNA in the IL-rich phases was analyzed to validate the method. This proposed process was subsequently used to extract plasmid DNA from bacteria and was compared with a commercially available kit. Further validation involved agarose gel electrophoresis and transformation of the extracted DNA into *E. coli*, which yielded promising results as shown in Figure 1.

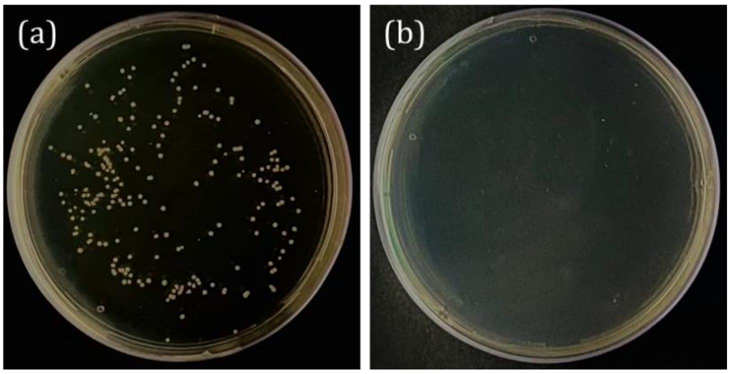


Fig. 1 : Result from the transformation experiment (a) of DNA obtained after extraction through ABS based extraction showing colonies and (b) control plate

While there is potential for improvement in DNA recovery and reusability of ABS, the described approach is comparable to conventional methods, cost-effective, and demonstrates a clear connection to sustainable processes.
in the future.

**References**

[1] N. Ali, R.D.C.P. Rampazzo, A.D.T. Costa, M.A. Krieger, *Biomed Res. Int.* (**2017)** 2017.

[2] S.P.M. Ventura, F.A.E. Silva, M.V. Quental, D. Mondal, M.G. Freire, J.A.P. Coutinho, *Chem. Rev.* (**2017**), 117, 6984–7052.

[3] K.K. Athira, R.L. Gardas, *Fluid phase equilib.* (**2022)** 558, 113463

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Effective Removal of Heavy Metal Ions using Hydrophobic Deep Eutectic Solvents

**M. SHAIBUNA, SACHIND PRABHA PADINHATTATH, RAMESH L. GARDAS***

Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036, India
*Corresponding author: e-mail: gardas@iitm.ac.in

**Keywords**: Hydrophobic deep eutectic solvent, Heavy metal ions, Wastewater treatment, Liquid-liquid extraction, Recycling

Toxic heavy metal ions (HMIs) in wastewater pose significant environmental and health risks. Conventional methods for their removal often lack efficiency, have high operational costs, and risk secondary pollution. Recently, Hydrophobic Deep Eutectic Solvent (HDES) based liquid-liquid extraction (LLE) has emerged as a promising alternative, offering enhanced selectivity and minimal secondary pollution. In this study, four novel HDESs were prepared by combining lidocaine or ibuprofen with heptanoic acid in various mole ratios to effectively remove toxic HMIs such as Cd(II), Pb(II), and Ni(II) from both stock solutions and mixtures, simulating real industrial conditions. The DESs were characterized using several spectroscopic and thermal techniques, and their physicochemical properties, such as density and viscosity, were studied concerning temperature. LLE experiments were conducted, and factors influencing the extraction process including metal ion concentration, volume ratio, and pH were meticulously optimized. Among the four HDESs, HDES1 (lidocaine-heptanoic acid at a 1:1 ratio) demonstrated superior performance, achieving over 95 % extraction efficiency in all cases. Additionally, stripping and reusability studies of HDES1 were performed, highlighting the sustainability and circular nature of the process.

## References

[1] C. Zamora-Ledezma, D. Negrete-Bolagay, F. Figueroa, E. Zamora-Ledezma, M. Ni, F. Alexis, V. H. Guerrero, Environ. Technol. Innov., 22 (**2021**) 101504.

[2] S. R. Dhokpande, S.M. Deshmukh, A. Khandekar, A. Sankhe, Sep. Purif. Technol., 350 (**2024**), 127868.

[3] N. A. A. Qasem, R. H. Mohammed, D. U. Lawal, NPJ Clean Water, 4 (**2021)** 1.

[4] M. Balali-Mood, K. Naseri, Z. Tahergorabi, M. R. Khazdair, M. Sadeghi, Front. Pharmacol., 12 (**2021**) 643972.

[5] D. Witkowska, J. Słowik, K. Chilicka, Molecules, 26 (**2021**) 6060.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Sustainable Metal Recovery from Spent Lithium-ion Battery Cathodes Using Deep Eutectic Solvents

**BAIJU CHENTHAMARA[1], RAMESH L. GARDAS[1*]**

[1]Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036, India
*Corresponding author: e-mail: *gardas@iitm.ac.in*

**Keywords**: Lithium-ion batteries, Deep eutectic solvents, Cathode recycling

Due to the abrupt accumulation of electrical and electronic wastes (WEEE) produced by quick technological advancements and the short lifespan of electronic gadgets[1]. In the modern technological world, the usage of lithium-ion batteries is inevitable due to their high energy density, which leads to over-demand and production. The overproduction expedites the formation of lithium-ion battery wastes, which are the prior source of $LiCoO_2$. Inorganic acids are employed in the hydrometallurgical leaching process to recover metals from discarded $LiCoO_2$ cathode materials, which has a detrimental effect on the environment. Deep Eutectic Solvents (DES) are a type of biocompatible solvents that emerged as a potential lixiviant for leaching applications[2]. Here we have designed a choline chloride-pyruvic acid -based DES as an effective alternative to the conventionally used inorganic acids for the leaching of $LiCoO_2$[3]. Differential Scanning Calorimetry (DSC) curves provide information on the eutectic composition and melting point of the prepared systems, and the reducing ability of HBD was studied using cyclic voltammetry. The high chloride content from the choline-based DES stabilizes the reduced $Co^{2+}$ by forming a blue color cobalt-chloro complex, which was proved by the UV-Visible spectroscopy[3]. As an extension of this, the molecular-level understanding of prepared DES has also been studied using DFT calculations.

## References

[1] N. Schaeffer, H. Passos, I. Billard, N. Papaiconomou, J.A.P Coutinho, Crit. Rev. Environ. Sci. Technol.,48 (**2018**), 859-922.
[2] L. Chen, Y. Chao, X. Li, Green Chem.,23 (**2021**), 2177-2184.
[3] B. Chenthamara, R. L. Gardas, ACS Sustain. Chem. Eng., xx (**2024**), xxxx-xxxx.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Solvent-Free Depolymerization Methods for Sustainable Plastic Waste Recycling into Value-Added products for Material Application

**MURUGESAN A[1]*, LOGANATHAN M, RAJENDRAPRASAD M**

[1]Polymer Science Engineering Lab, Department of Chemistry, Sri Sivasubramaniya Nadar College of Engineering, Kalavakkam- 603 110, India
*Corresponding author: e-mail: murugesana@ssn.edu.in

**Keywords**: polyethylene terephthalate, thermal analysis, DSC, TGA, triphosgene, energy application

## Abstract:

The increasing global demand for sustainable plastics recycling has driven research into innovative depolymerization processes. This study explores the thermocatalytic depolymerization (TCDP) of polyethylene terephthalate (PET) and polycarbonate (PC) at 200 ℃ using ethylene glycol (EG) and Yttrium Oxide ($Y_2O_3$) as catalysts. $Y_2O_3$ facilitated the conversion of EG into cyclic ethylene oxide (CEO) and broke polymer bonds, yielding Bis(2-hydroxyethyl) terephthalate (BHET) and Bisphenol A (BPA) with 80% and 83% recovery, respectively. Recovered monomers were used to synthesize polycarbonate and co-polycarbonate (Co-PC) via polycondensation with triphosgene. The structural integrity of the monomers and polymers was confirmed through Fourier Transform Infrared Spectroscopy (FTIR), Nuclear Magnetic Resonance (NMR), and X-ray Diffraction (XRD). Thermal properties assessed by thermogravimetric analysis (TGA) revealed degradation temperatures of 420 ℃ for PC and 442 ℃ for Co-PC, indicating a 22 ℃ increase for Co-PC, demonstrating enhanced thermal stability.

Additionally, a solvent-free melt depolymerization process was employed to recover BHET from PET waste, which was further hydrolysed to produce terephthalic acid (r-TPA). Both r-BHET and r-TPA were utilized to construct cerium-based metal-organic frameworks (MOFs) for potential energy applications. Extensive characterization, including FTIR, NMR, Field Emission Scanning Electron Microscopy (FE-SEM), and Energy-Dispersive X-ray Spectroscopy (EDX), confirmed the structural integrity and purity of r-BHET, r-TPA, and the synthesized MOFs. The specific capacitances of r-BHET and TPA-Ce-MOF were measured at 91.5 and 220.125 F/g, respectively.

### References

[1] Smith, R. L, Takkellapati, S, Riegerix, R. C, ACS Sustainable Chem. Eng., 10 (2022), 2084–2096.
[2] Marullo, S, Rizzo, C, Nadka Tzankova Dintcheva, D’Anna, F, ACS Sustainable Chem. Eng., 9 (2021), 15157–15165.
[3] Iannone, F, Casiello, M, Monopoli, A, Cotugno, P, Sportelli, M. C, Picca, R. A, Cioffi, N, Dell’Anna, M. M, Nacci, A, Journal of Molecular Catalysis A: Chemical, 426 (2017), 107–116.

T8- PP 05

# Fe-doped Zinc-MOF Composites and its Test-Strip Employed for Colorimetric Detection of Glucose in Model and Real Urine Samples

**Vibhav Shukla[1], Kafeel Ahmad Siddiqui[1]***

[1] Department of Chemistry, National Institute of Technology, Raipur, C.G. 492010, India
*Corresponding author: e-mail: *vshukla.phd2022.chy@nitrr.ac.in*

**Keywords**: Metal Organic Framework, MOF-Composite, Detection of Glucose, Urine Sensing.

We present an innovative luminescent probe based on a novel Metal-Organic Framework (MOF), {[Zn3(Cei)2(COO)2(Bimb)3]·C2H2}n (Zinc-MOF), and its iron-doped composite (Fe@Zinc-MOF), meticulously designed for glucose detection. The structural integrity and performance of these composites were validated through comprehensive analytical techniques. The probe demonstrated exceptional linear correlation coefficients ($R^2 = 0.97118$) for glucose concentrations of 110 and 150 mg/dl. Impressively, the Stern-Volmer quenching constants (Ksv) at low glucose concentrations were determined to be $3.2 \times 10^4\ M^{-1}$ and $3.8 \times 10^4\ M^{-1}$ in real urine samples. The probe achieved remarkable detection limits of 1.17 ppm and 0.846 ppm for 110 and 150 mg/dl glucose, respectively, in real urine samples. To further enhance practicality, a highly sensitive detection strip was fabricated using filter paper impregnated with the Fe@Zinc-MOF composite. This strip exhibited significant fluorescence changes corresponding to varying glucose concentrations, underscoring its potential for ultra-sensitive glucose monitoring. Our findings pave the way for advanced, real-time glucose detection in clinical diagnostics, offering a promising tool for efficient health monitoring.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Biodegradable and sustainable PLA-based substrates destined for printed and flexible electronics

**NIKOLAOS D.BIKIARIS[1]*, RAFAIL IOANNIDIS[1], NIKOLAOS NIKOLAIDIS[1]**

[1] Department of Chemistry, Aristotle University of Thessaloniki, GR-541 24 Thessaloniki, Greece
*Corresponding author: e-mail: nbikiaris@gmail.com

**Keywords**: printed electronics, PLA, copolymers, thermal properties

Printed, flexible, and hybrid electronic technologies are developing rapidly leading to remarkable developments in smart wearables, sensor applications, and health monitoring systems [1]. In the light of global environmental concerns regarding fossil raw materials, there is a necessity to drive the production of flexible electronics devices based on sustainable materials. Moreover, there is a need to reduce the quantity of electronic waste by developing material recovery and recycling technologies. The only mass-produced polymer that is simultaneously biocompatible, potentially biodegradable, and biobased is PLA, which has the highest manufacturing capacity among biobased polymers [2,3]. When it comes to manufacture, PLA is more advantageous than traditional polymers since it is mostly formed of cellulose, starch, maize, and waste materials.

The main goal of the present work is to overcome the limitations of PLA by the synthesis of novel copolyesters from renewable resources. Novel poly(lactic acid)-b-poly(ethylene azelate) copolyesters were synthesized via ring opening polymerization (ROP) of l-lactide, and their properties were studied through various techniques. The presence of the second comonomer within the macromolecular chains of PLA caused only a slightly decreased 10 °C towards lower temperatures, while glass transition temperature and cold crystallization temperature of the copolymers shifted up to 20 and 35 °C, respectively. The copolyester with 20 wt% of PEAz segments, exhibited two glass transition temperatures, indicating the formation of block copolyesters. Because printed electronics (PE) could be one of the potential application for these innovative copolyesters, their high melting temperatures are crucial for applying high curing temperatures (120 – 130°C) during the printing experiments.

**Acknowledgements**

This work was funded from the European Union's HORIZON 2020 Research and Innovation Actions Program under Grant Agreement No. 101070556 (Sustain-a-Print Project).

**References**

[1] Luoma, E., Välimäki, M., Ollila, J., Heikkinen, K., & Immonen, K. (2022). Bio-based polymeric substrates for printed hybrid electronics. Polymers, 14(9), 1863.
[2] https://www.european-bioplastics.org/market/.
[3] E. Balla, V. Daniilidis, G. Karlioti, T. Kalamas, M. Stefanidou, N.D. Bikiaris, A. Vlachopoulos, I. Koumentakou, D.N. Bikiaris, Polymers. 2021, 13, 1822.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Investigating Experimental and Theoretical Thermophysical Properties of Binary Systems of Deep Eutectic Solvents with Water

**VAHISHTA KATRAK[1]*, SUSHMA P. IJARDAR [2]**

[1]Research Scholar, Department of Chemistry, Veer Narmad South Gujarat University, Surat
[2]Assistant Professor, Department of Chemistry, Veer Narmad South Gujarat University, Surat 395007, India
*Corresponding author: E-mail: sijardar@vnsgu.ac.in

**Keywords**: deep eutectic solvents (DESs), binary mixtures, excess molar volume, excess molar compressibility, PFPT & ERAS

In modern green chemistry, Deep eutectic solvents (DESs) have gained appreciable recognition as an analog of ionic liquids (ILs) due to their inexpensive and easy-to-handle preparation method. DESs exhibit similar physio-chemical properties to ILs and are considered as a suitable alternative to volatile organic solvents [1]. In this work, the densities, and speeds of sound of binary mixtures formed by alkyl triphenyl phosphonium bromide-based DES with water have been determined over the whole range of composition at the temperature range from 298.15 to 313.15 K and at atmospheric pressure using a vibrating-tube densimeter (DSA 5000) [2]. The Excess molar volumes and excess isentropic compressibilities have been obtained from these experimental results, and have been fitted by the Redlich-Kister equation. The stronger interaction between water and components of studied DESs gave negative values for both excess molar properties. This behavior of the investigated systems was assessed using the Extended Real Associated Solution Model (ERAS) and Prigogine-Flory-Patterson theory (PFPT) [3,4,5]. The results have been interpreted in terms of ion-dipole interactions and structural factors of ion-dipole interactions and structural factors of the DES and water.

**References**

[1] R. Sharma, K.K. Athira, R. L. Gardas, N. Malek, S. P. Ijardar, *Journal of Molecular Liquids*, 367 (**2022**) 120386.
[2] J.A. Widegren, J.W. Magee, *Journal of Chemical & Engineering Data,* 52 (**2007**) 2331-2338.
[3] H. Shekaari, M.T. Zafarani-Moattar, M. Mokhtarpour, S. Faraji, *Journal of Molecular Liquids,* 289 (**2019**) 11077.
[4] M. Mokhtarpour, H. Shekaari, *Journal of Molecular Liquids,* 320 (**2020**) 114224.
[5] B. Nowosielski, M. Jamrogiewicz, J. Luczak, M. Smiechowski, D. Warminska, *Journal of Molecular Liquids,* 309 (**2020**) 113110.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Designing Aqueous Biphasic Systems of Quaternary Ammonium Salt based Deep Eutectic Solvents in presence of Inorganic Salts

**NENSI PATEL[1]*, SUSHMA P. IJARDAR[2]**

[1]Research Scholar, Department of Chemistry, Veer Narmad South Gujarat University, Surat
[2]Assistant Professor, Department of Chemistry, Veer Narmad South Gujarat University, Surat
395007, India
*Corresponding author: E-mail: sijardar@vnsgu.ac.in

**Keywords**: deep eutectic solvents (DESs), aqueous biphasic systems (ABSs), inorganic salts

The newest solvent to join the eco-friendly solvent family is deep eutectic solvents (DESs) [1]. The application of DESs has become one of the major strategies in green chemistry. DESs have been introduced in aqueous biphasic systems (ABSs) owing to lower cost of starting material, ease of preparation, higher tunability and biodegradability, have led to a new trend within the scientific community and industry [2,3]. In this work, ABSs formed by different DESs and inorganic salts at 25 °C were examined. The DESs were prepared from benzyl trialkyl ammonium chloride salts (i.e. hydrogen bond acceptors) and Polyethylene glycol (i.e. hydrogen bond donors). The obtained DESs were used to form ABSs with inorganic salts by employing cloud point titration method. Empirical non-linear expression developed by Marchuk et al. was used to fabricate the binodal curves while the tie lines were determined using Othmer-Tobias and Bancroft equations [4]. Phase-forming capacity of the salts, alkyl chain length of HBA and HBD were also investigated in addition to factors affecting phase formation.

**References**

[1] A.P. Abbott, G. Capper, D.L. Davies, R.K. Rasheed, V. Tambyrajah, *Chemical Communications*, 22 (**2003**) 70–71.
[2] R. Sharma, K.J. Jisha, R.L. Gardas, N. Malek, S.P. Ijardar, *Journal of Molecular Liquids*, 366 (**2022**) 120278.
[3] E. A Oke, S. P Ijardar, *Journal of Molecular Liquids*, 375 (**2023**) 121372.
[4] Y. Marcus, *Journal of the Chemical Society, Faraday Transactions*, 87 (**1991**) 2995-2999.

# Elucidating Molecular Interactions of Imidazolium-Based Ionic Liquid in Aqueous and Aqueous Amino Acid Solutions: Volumetric and Compressibility Studies

**ANUJA JAIN, VANDANA PATEL, SANGESH P. ZODAPE***

Department of Chemistry, Visvesvaraya National Institute of Technology (VNIT), Nagpur- 440 010,
Maharashtra, India
*Corresponding author: e-mail: szodape@chm.vnit.ac.in, sangesh02@gmail.com

**Keywords:** Density; Speed of sound; Ionic liquid; Amino acid; Limiting apparent molar volume; Limiting apparent molar isentropic compressibility.

Imidazolium Ionic liquid (IL), known for their distinct features and numerous applications, were chosen for their importance in domains like as biology, pharmaceutical chemistry and green chemistry. To achieve a detailed understanding of interactions, we conducted precise density and sound velocity measurements within concentration 0.01-0.15 kg.mol$^{-1}$ at different temperatures i.e. 293.15, 298.15, 303.15, 308.15, and 313.15 K. These measurements allowed us to determine key parameters, including the apparent molar volume of the solute ($V\phi$), limiting apparent molar volume of solute ( $V^{o}_{\phi}$ ) , isentropic compressibility of solution( $\kappa S$ ), apparent molar isentropic compressibility of solute ( $KS\ ,\phi$ ) , limiting apparent molar isentropic compressibility of the solute ( KS. $^{o}_{\phi}$ ) and the limiting apparent molar expansivity of solute ($E^{o}_{\phi}$) for studied systems at different temperatures. Our findings in studied systems show strong solute-solvent interactions, as seen by the creation of structured hydration shells around the IL ions. In ternary system, the type of the side chains (hydrophilic, hydrophobic, or amphiphilic) of the amino acid further influences the molecular interactions. The compressibility results reveal that the addition of amino acid decreases the compressibility of the studied system, reflecting a more organized and less compressible environment.

## References

1. Jain, A., Shende, V. S., Kawadkar, D. V., Pratap, U. R., Wankhade, A. V., Zodape, S. P., J. Chem. Thermodyn. 2021, 162, 106561.
2. Jain, A., Zodape, S. P., J. Mol. Liq. 2022, 363, 119817.
3. Jain, A., Zodape, S. P., J. Chem. Eng. Data, 2023,68(8),1899–1910

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Apparent Molar Volumes and Apparent Molar Isentropic Compressibilities of Procaine/Tetracaine Hydrochloride in Aqueous Solutions at Different Temperatures

**MUSTAQUEEM M. SHAIKH[1], SANGESH P. ZODAPE[2], VANDANA PATEL[2], VASIM R. SHAIKH[1*]**

[1]School of Chemical Sciences, K. C. E. Society's Moolji Jaitha College (Autonomous),
Jalgaon-425001, Maharashtra, India.
[2]Department of Chemistry, Visvesvaraya National Institute of Technology, Nagpur–440010,
Maharashtra, India
*Corresponding author: vasimshaikh84@gmail.com

**Keywords**: local anesthetical drug, procaine hydrochloride, tetracaine hydrochloride, apparent molar volume, apparent molar isentropic compressibility

The experimental measurements of density and speed of sound for the two local anesthetical drugs, namely, procaine hydrochloride PC·HCl (0.04566 – 0.30021 mol·kg−1) and tetracaine hydrochloride TC·HCl (0.04476 – 0.30127 mol·kg−1) in aqueous solutions at T = 288.15, 293.15, 298.15, 303.15, 308.15, 313.15 and 318.15 K are reported. Further, density and speed of sound data used to calculate apparent molar volume and apparent molar isentropic compressibility of PC·HCl and TC·HCl at the finite concentrations as well as apparent molar volume at the infinite dilute solution and apparent molar isentropic compressibility at the infinite dilute solution. The coefficient of thermal expansion of solutions, apparent molar expansibility of solute at the finite concentration and apparent molar expansibility of solute at the infinite dilution were also calculated at 293.15, 298.15, 303.15, 308.15, 313.15 K. All these results are analysed and discussed on the basis of solute-solvent and procaine/tetracaine cation-cation interactions in aqueous solutions.

## References

[1] H. Matsuki, S., Hashimoto, S. Kaneshina and M. Yamanaka, *Langmuir* 10 (**1994**) 1882.
[2] D. R. Delgado, A. F. Jimenez–Kairuz, R. M. Manzo, E. F. Vargas and F. Martinez, *Rev. Colomb. Cienc. Quim. Farm.* 39 (**2010**) 57.
[3] V. R. Shaikh, D. H. Dagade, D. G. Hundiwale and K. J. Patil, *J. Mol. Liq.* 164 (**2011**) 239.

# Thermodynamic studies of maline (choline chloride + malonic acid) and ethanol based pseudo-binary mixture

**SAPNA R. WARKARI[1]*, NIRAJ T. KHATY[2], VIJAY M. TANGDE[2], SUDHAKAR S. DHONDGE[3].**

[1] Department of Chemistry, Rashtrasant Tukadoji Maharaj Nagpur University, Nagpur-440033, India
[2] Laxminarayan Innovation Technological University, Nagpur-440033, India
[3] Department of Chemistry, S. K. Porwal College, Kamptee-441001, India *Corresponding author: e-mail: sapna.warkari@gmail.com

**Keywords**: Deep eutectic solvent (DES), Hydrogen bond acceptor (HBA), Hydrogen bond donor (HBD), Thermophysical parameters.

The present study reports the densities, speed of sound and viscosities of Deep eutectic solvent (DES) named as maline comprising of an equimolar mixture of choline chloride as hydrogen bond acceptor (HBA) and malonic acid as hydrogen bond donor (HBD) in the presence of ethanol with different concentrations at seven different temperatures (293.15 K- 323.15 K) with an interval of 5K. Using the corresponding data, different thermophysical parameters like excess molar volume $(V^E)$, excess isentropic compressibility $(K_s{}^E)$ , excess intermolecular free length $(L^E{}_F)$ , deviation in viscosity $(\Delta_\eta)$, excess speed of sound $(u^E)$, excess acoustic impedance $(Z^E)$, and surface tension were calculated to study the effect of temperature and varying mole fraction. Additionally, the study also signified the favorable hydrogen bonding interactions between maline and ethanol have been illustrated[1], [2].

**References**

[1] A. K. Jangir, A. K. Nain, and K. Kuperkar, *J Mol Liq*, 334, (**2021**)
[2] J. Naser, F. S. Mjalli, and Z. S. Gano, *J Chem Eng Data*, 61 (**2016**) 1608–1615.

**T10- PP 06**

# Delving into solutions of Azithromycin in 1,2-propanediol, DMSO and ethanol through ultrasonic, volumetric and viscometric properties analysis across a temperature range of 288.15 K to 318.15 K

**SNEHA BANKAR[1]*, PRANALI UMREDKAR[1], APARNA KHATY[1], VIJAY TANGDE[1], NIRAJ KHATY[2], SUDHAKAR DHONDGE[3]**

[1]Department of Chemistry, Rashtrasant Tukadoji Maharaj Nagpur University, Nagpur 440033
[2] Department of Chemistry, Laxminarayan Innovation Technological University 440033
[3]Department of Chemistry, S. K. Porwal College, Kamptee 441001
*Corresponding author: stbankar7@gmail.com

**Keywords:** apparent molar volume, azithromycin, Jones-Dole coefficient, 1,2propanediol, DMSO

The densities, speed of sound and viscosities in binary mixtures consisting of Azithromycin with 1,2-propanediol, DMSO and ethanol were extensively measured across the concentration (0.02 mol.kg-1 -0.1 mol.kg-1 ), ranging from 288.15 K to 318.15 K with 5 K intervals. Utilizing the gathered experimental data, the apparent molar volume of solute V, limiting apparent molar volume of solute ($V\phi^0$), isentropic compressibility of solution ($\kappa s$) , apparent molar isentropic compression of the solute (K ) , limiting apparent molar isentropic compressibility of solute ($Ks\phi^0$ )and apparent molar expansibility of solute($E\phi^0$). Further, the coefficient of thermal expansion ($\propto^*$) , the second-order derivative of limiting apparent molar volume ($\partial^2 V\phi^0/\partial T^2$), Jones-Dole equation viscosity A, B, D coefficients, temperature derivative of B coefficient i.e. (dB/dT), activation parameters for viscous flow were computed for these examined mixtures. The outcomes were evaluated based on molecular interactions and structural impacts. The results are analyzed in terms of the nature of solute-solvent interactions. The positive apparent molar volume of the solute indicates strong hydrogen bonding between the drug and solvent. The strength of this hydrogen bonding increases with higher concentration and temperature [1], [2].

## References

[1] M. J. Liu et al., J. Mol. Liq.,199 (2014) 51–56.
[2] N. P. Mohabansi, A. K. Satone, and S. N. Hirani, Russ. J. Phys. Chem. A, 95 (2021) S1–S7.

# Elucidation of molecular interactions in cyclohexanol with aniline and chloro substituted aniline binary mixtures in terms of spectroscopic and DFT study

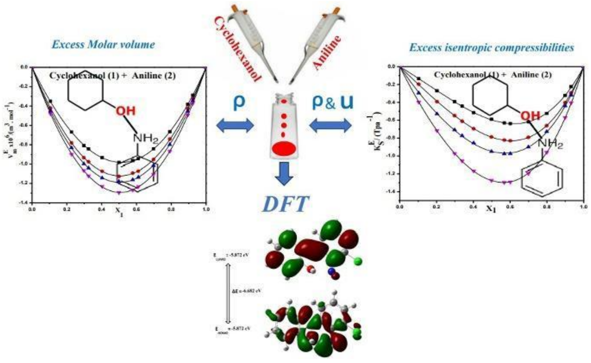
**E. A. LOHITH[1]*, K. KEERTHI[1], S. RAVIKUMAR[2], R. KARTHIK[2], K. SIVAKUMAR[3*], N. V. V. JYOTHI[1]**

[1] Department of Chemistry, Sri Venkateswara University, Tirupati 517502, India
[2] Department of Physics, Saveetha School of Engineering, SIMATS University, Chennai-602105, India
[3] Department of Chemistry, S. V. Arts College, T.T.D, Tirupati 517502, India
*Corresponding author: e-mail: sivakumarkasi64@gmail.com

**Keywords**: excess properties, molecular interactions, structural effects, FT-IR, DFT

Density $(\rho)$ and sound speed $(u)$ findings on the binary liquid mixtures consisting of cyclohexanol (CH-OH), with aniline (A), *ortho*-chloroaniline (*o*-CA), and *meta*-chloroaniline (*m*-CA) were gathered at the various temperatures spanning the entire concentration range. 303.15, 308.15,313.15, and 318.15 K at atmospheric pressure. The measured Information was utilized to compute excess molar volume $(V_m^E)$, excess isentropic compressibility $(K_s^E)$, excess of speed of sound $(u^E)$, excess intermolecular free length $(L_f^E)$ and excess acoustic impedance $(Z^E)$. Further, the partial molar volumes $(\bar{V}^\circ_{m,1}.\bar{V}^\circ_{\varphi,1}.\bar{V}^\circ_{m,2}.\bar{V}^\circ_{\varphi,2})$, partial molar compressibilities $(\bar{K}^\circ_{m,1}, \bar{K}^\circ_{\varphi,1}, \bar{K}^\circ_{m,2}, \bar{K}^\circ_{\varphi,2})$ and their excess values $(\bar{V}^E_{m,1}.\bar{V}^{\circ E}_{\varphi,1}.\bar{V}^E_{m,2}.\bar{V}^\circ_{\varphi,2})$, $(\bar{K}^E_{m,1}, \bar{K}^\circ_{\varphi,1},\bar{K}^E_{m,2}, \bar{K}^\circ_{\varphi,2})$ were also computed to perceive more information on molecular interaction and structural effects in these mixtures. Applying the theory of Prigogine-Flory- Patterson (PFP) as a framework, the $(V_m^E)$ data of the current liquid mixtures were examined. The analysis of the experimental data considered the interactions between the individual molecules that make up liquid mixtures. By using the Density Functional Theory (DFTB3LYP) of 6-311 ++ G to analyze the geometries, bond characteristics, interaction energies, and hydrogen bonded complexes in organic solvent phase, quantum chemical calculations were able to further confirm the hydrogen bonding that predominates between cyclohexanol with aniline and chlorosubstituted anilines.

**Graphical abstract**



*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

---

# Temperature Effects on Physicochemical and Thermodynamic Properties of Natural Deep Eutectic Solvents (NADES) and their Aqueous Mixtures

**OMISH SETHI[1], ASHWANI KUMAR SOOD[1], TEJWANT SINGH KANG[1,*]**

[1]Department of Chemistry, UGC Centre for Advance Studies-II, Guru Nanak Dev University,
Amritsar, Punjab-143005, India
*Corresponding author: e-mail: tejwant.chem@gndu.ac.in

**Keywords**: Deep Eutectic Solvents, Thermal Stability, Walden Plot, Cytotoxicity

Today, DESs are widely recognized as a novel class of sustainable solvents representing a green alterative to ionic liquids (ILs). Natural Deep Eutectic Solvents (NADES) are generally composed of components that are abundant in our daily diet, such as choline, amines, sugars, polyalcohols, and carboxylic acids. NADES fully fit the principles of green chemistry and offer many advantages, including low cost, readily available component, simple preparation, and a low toxicity profile. The binary mixtures of DESs with water are attracting a great deal of interest for various industrial applications owing to their unique properties not exhibited by the neat components.[1,2] Therefore, the thermodynamic properties of NADES-water mixtures should be explored to better understand the prevailing intermolecular interactions for enhancing the application arena of such binary mixtures.

NADES have been thoroughly characterized and investigated for their physicochemical properties, viz. thermal stability, viscosity ($\eta$), refractive index ($n_D$), density ($\rho$), speed of sound (u), and conductivity ($\kappa$) at different temperatures and atmospheric pressure. The thermal stability of the NADES has been investigated using the thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) techniques, respectively. The influence of temperature, type of HBDs, and alkyl chain length of HBDs in the NADES on the physicochemical properties is critically examined and discussed. The values of various thermodynamic parameters have been derived and discussed in terms of the varying extent of intermolecular interactions governed by the components of DESs. A relationship between molar conductivity and dynamic viscosity (Walden Plot) has been established to evaluate the ionicity of the synthesized NADES. Further, this work also aimed to explore the cytotoxic profile of NADES systems with different hydrogen bond donors (HBDs).

**References**

[1] O. Sethi, M. Singh, T. S. Kang, and A. K. Sood, *Journal of Molecular Liquids* 340 **(2021)** 117212.
[2] O. S. Hammond, D. T. Bowron, K. J. Edler, *Angewandte Chemie International Edition* 56 **(2017)** 9782–9785.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Influence of Mono- and Di-cationic Ionic Liquids on Bile Salt Aggregation and Drug Interaction

**V. P. PRIYANKA[1], RAMESH L. GARDAS***
[1] Department of Chemistry, Mar Ivanios College, Thiruvananthapuram-695015, India
* Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036, India
*Corresponding author: e-mail: gardas@iitm.ac.in

**Keywords**: Monocationic Ionic Liquids, Dicationic Sodium deoxycholate, Mixed micellar system; Aggregation behavior; Ciprofloxacin

Ionic liquids (ILs) are valued for their unique properties, such as low vapor pressure, thermal and chemical stability, and the ability to tune their characteristics by selecting different anions and cations, making them important in chemistry and biology [1]. ILs can also exhibit surface-active properties, which opens up various therapeutic applications. However, many drugs have poor water solubility, leading to reduced effectiveness in biological systems. Surfactants, known for their aggregation properties, help solubilize poorly soluble drugs by incorporating them into micellar systems [2, 3]. Bile salts, a biological surfactant, enhance the solubility and bioavailability of hydrophobic drugs in water [4]. Compared to traditional surfactants, the binary mixture of ILs and bile salts (mixed micellar system) exhibits improved surface characteristics [5].

This study focuses on the aggregation behavior of sodium deoxycholate (a bile salt) in water and in aqueous solutions of imidazolium-based mono- and di-cationic ILs. The critical micellar concentration (CMC) was determined using conductivity and fluorescence experiments. The results showed that ILs decrease the CMC of sodium deoxycholate, indicating enhanced surface properties. The system with a hydrophobic mono-cationic IL had a lower CMC, suggesting a stronger affinity for the bile salt. As the IL concentration increased, the CMC decreased, confirming easier aggregation. The mixed micellar system containing 0.15 wt% ILs, which could form larger aggregates and lower CMC, was chosen for the interaction study with ciprofloxacin and the interaction parameters were analyzed using the Benesi-Hildebrand equation. It was observed that the mixed micellar system containing hydrophobic IL exhibited the highest binding affinity towards CIP.

## References

[1] V. P. Priyanka and R. L. Gardas, Sep. *Purif. Technol*, 234 (**2020)** 116048.
[2] R.Vashishat, R. Sananb, and Mahajan, R. K. *RSC Adv*, 5 (**2015**) 72132-72141.
[3] M. K. Banjare, K. Behera, R. Kurrey, R. K. Banjare, M. L. Satnami, S. Pandey, and K. K. Ghosh, *Spectrochim. Acta A Mol. Biomol. Spectrosc*, 199 (**2018)** 376-386.
[4] S. J. Selvam, S. *J. Photochem. Photobiol, B*, 116 (**2012**) 105-113.
[5] R. S. Makkar, and K. J. Rockne, *Environ. Toxicol. Chem*, 22 (**2003)** 2280-2292.

*18th International Congress on Thermal Analysis and Calorimetry, IIT Madras, India, 02-07 Sept. 2024*

# Investigating Hemoglobin Stability in DBU-Based Protic Ionic Liquids: A Spectroscopic Approach

**K. J. JISHA[1], RAMESH L. GARDAS***
[1] Department of Chemistry, St Mary's College, Sulthan Bathery- 673592, India
* Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036, India
*Corresponding author: e-mail: gardas@iitm.ac.in

**Keywords**: DBU, Ionic liquid, Hemoglobin, Cosolvent, Solubility, Structural stability

Proteins, as biopolymers formed by amino acid condensation, must maintain a stable structure, crucial for their function in therapeutics, biological processes, and diagnostics. Globular proteins, like heme proteins, achieve stability through a balance of intermolecular interactions and co-solvent effects, which influence protein rigidity and flexibility based on the solvent's polarity [1]. The choice of an appropriate solvent is key in both academic and industrial settings for biomolecule applications. Among various additives, Ionic Liquids (ILs) have emerged as favorable due to their thermal stability, low vapor pressure, and reusability, making them ideal for protein separation, extraction, and preservation [2,3]. The interaction of proteins with ILs varies, with ILs capable of acting as both stabilizers and denaturing agents depending on the conditions. It's noteworthy to note that, depending on the protein molecule it is interacting with, each protein behaves differently according to the properties of the ionic liquids [4,5].

DBU-based ILs, synthesized with Imidazole, Morpholine, and Triazole, are notable for their high thermal stability but are less explored in biomolecular applications. This study investigated the interaction of these ILs with hemoglobin using techniques like UV-Visible spectroscopy, fluorescence, and dynamic light scattering. The results indicated that all three IL systems were hemoglobin-friendly, with the Triazole system being particularly effective. The binding constant values showed no complex formation during IL-Hb interactions, confirming that these ILs can serve as suitable co-solvents for hemoglobin-like proteins, offering a medium that supports protein stability without interfering with critical intermolecular interactions.

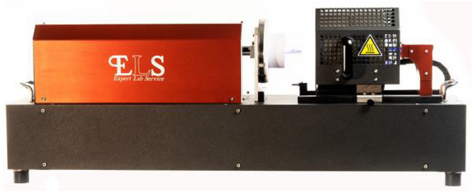
**References**

[1] I. Jha, P. Attri, and P.Venkatesu, *Phys. Chem. Chem. Phys*. 16 (**2014**) 5514–5526.
[2] T. Welton, *Biophys Rev*. 10 (**2018**) 691–706.
[3] M. Guncheva, *Protein Journal*. 41 (**2022)** 369–380.
[4] A. Schindl, M. L. Hagen, S. Muzammal, H. A. D. Gunasekera, and A. K. Croft, *Front. Chem*. 7 (**2019)** 347.
[5] C. Schröder, *Top Curr Chem*. 375 (**2017)** 25.

# ELICO MARKETING PVT. LTD

## Discover our tools for Thermal Analysis

### ELS-MDF: Microscope & Optical Dilatometer



ELS-MDF is the new contact-less optical thermal analysis instrument able to reproduce heating cycles by unifying the following measurement techniques:

Heating Microscope : Fusibility (raw materials, glazes, frits, ashes,glass)
Optical Dilatometer: CTE , glass transition temperature, volume variation, sintering , softening point;
Optical Fleximeter : Piroplasticity and the state of tension between layered materials.

### IMCE Resonant Frequency Damping Analyzer

Material characterization at high temperatures
The Resonant Frequency and Damping Analyser (RFDA) is based on the impulse excitation technique (IET). This is a non-destructive material characterization technique to measure the elastic properties of a material.

This dynamic test method uses the resonant frequencies, sample dimensions and mass to determine Young's modulus, shear modulus, Poisson's ratio and damping/internal friction.
Available to perform from -100°C up to maximum 1700°C

### THERMTEST Thermal Conductivity Analyzer

The MP-1 is designed to test the absolute thermal conductivity, thermal diffusivity and specific heat of solids, liquids, pastes and powders with the powerful combination of the Transient plane source (TPS, ISO 22007-2) , Transient hot-wire (THW, ASTM D7896), Transient Line Source (ASTM D5334) , MTPS and Transient Hot Strip (THS).

Best for Solids, Liquids, Pastes, and Powders.
Thermal Conductivity 0.005 to 1800 W/m•K
Extended Temperature Range -160 to 1000 °C

### THERMTEST Heat Flow Meter

Heat flow meter for measuring the thermal conductivity and thermal resistance of insulation, Textiles , construction materials. HFM 100 is designed for testing both homogeneous and heterogeneous materials. Follows ASTM C518, ISO 8301.

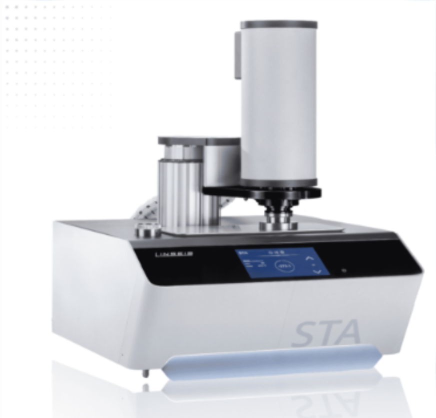
| | |
|---|---|
| Materials | Insulation, Solids, and Textiles |
| Direction | Through-Thickness |
| Thermal Conductivity Range | 0.002 to Up to 2.5 W/m•K |
| Plate Temperature Range** | -30 to 110 °C |

### THERMTEST Guarded Heat Flow Meter

The Guarded Heat Flow Meter (GHFM-01) follows ASTM E1530-19 for thermal resistance and thermal conductivity of solids, such as metals, polymers, composites and paste. The Thermtest proprietary testing stack, replaces the traditional pneumatic movement with advanced motor control.

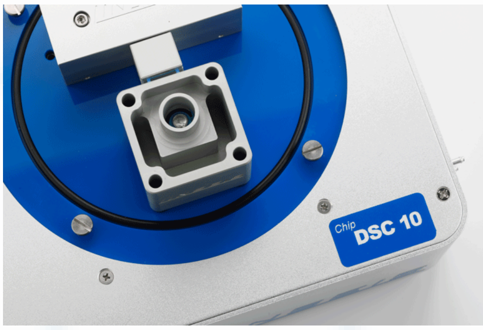
Full computer control : Mean temperature, sample thickness, force / pressure applied.
Programmable mean temperatures from -20 °C to 310 °C.
hickness is measured to an accuracy of 0.0254 mm, with use of a digital optical encoder.

All new DSC PT 1000



STA with patented Forced Flow Technology

Introducing Isothermal Battery Calorimeter (IBC)



Chip DSC

Thermogravimetric Analyzer


C-THERM


NETZSCH
ARC 244
DSC 300 Caliris
NETZSCH
TG 309 Libra
NETZSCH

शिक्षा मंत्रालय
MINISTRY OF
**EDUCATION**

सत्यमेव जयते

# SWAYAM PRABHA

(An initiative by Ministry of Education)

SWAYAM PRABHA
Free DTH Channel for Education

SWAYAM PRABHA is a group of 40 channels devoted to telecasting of high-quality educational programmes on 24X7 basis using the GSAT-15 satellite. With atleast 4 hours of fresh content repeated about 5 times daily, students have the privilege of choosing the viewing time as per their convenience. Content creation is coordinated by IITs, CEC, IGNOU & UoH. BISAG-N is responsible for uplinking the 40 DTH channels. INFLIBNET Centre maintains the SWAYAM PRABHA web portal.

## Our Partners

www.swayamprabha.gov.in

BISAG-N MeitY Engineering to Imagineering | ignou THE PEOPLE'S UNIVERSITY | CEC | TIRUPATI

- With atleast 4 hours of fresh content repeated about 5 times daily, students have the privilege of choosing the viewing time as per their convenience
- Content creation is coordinated by IITs, CEC, IGNOU & UoH.
- BISAG-N uplinking the 40 DTH SWAYAM PRABHA channels
- INFLIBNET centre maintains the SWAYAM PRABHA web portal
- 1.2 Lakhs + videos cover curriculum based course contents of UG/PG level of divers discipline including technical, non-technical & competitive exams
- SWAYAM PRABHA channels can be accessed through DDFree Dish|Dish TV| JiO Mobile App
- Archive videos & programme schedule for all channels
- Learn from eminent professors at your home
- IIT PAL: To assist the students for classes 11 and 12, who are aspiring to join IITs

**Telecasting high-quality educational programmes 24/7**

**Breaking Down Barriers to Education with Swayam Prabha**

**Connect with us using WhatsApp Service**

LIVE STREAMING | DD Free Dish | dishtv | Jio Mobile App

follow us

**Office of the Chief Coordinator**
**MSB 150, Department of Chemical Engineering**
**Indian Insttitute of Technology Madras**
**Chennai - 600036**

# Green Chemistry Letters and Reviews

*An international, cross-disciplinary, fully open access journal focused on the contribution of chemistry to sustainable development.*

*Green Chemistry Letters and Reviews* covers the following topics: green synthesis and catalysis, green manufacturing and engineering, green product design, green chemistry education, critical raw materials and sustainable resources, and energy harvest, storage, and savings.

We are interested in original research articles, research and education letters, research and education reviews, and comments.

**We welcome your submissions!**

https://www.tandfonline.com/journals/tgcl20

Taylor & Francis Group
an **informa** business

Rigaku

Differential Scanning Calorimeter

# DSCvesta2

## New Xsensor

with both high sensitivity and toughness

**Improved measurement reproducibility**

- Noise level of 0.05 μW realized
- Capable of measuring temperatures up to 600°C in atmospheric conditions.

### Equipped with the industry's First self-diagnostic function, vestaeye

Continuously monitors equipment status and contributes to reliable daily measurements through preventive maintenance

**NEW**

- Unparalleled temperature range (-180 to 725℃)
- Don't miss even the slightest changes with low noise & state-of-the-art sensors
- Observe your samples in real time with live imaging during measurements
- Always self-diagnosing with the cutting-edge vestaeye feature

DSCvesta2
▶WEB page