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Inaugural of Schrodinger Material Science Workshop | Pg. 8 National Conference AMES- 2023 | Pg. 10

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From the HOD's Desk

Dear Readers,

I am glad to present the January 2024 issue of our department's newsletter. In this issue, we showcase the latest updates and accomplishments and highlight the talent and dedication within our department. You will find insightful articles, research updates, faculty and student achievements, and exciting event highlights on these pages. I encourage you to read, engage, and share your thoughts.

I am pleased to inform you that we had an MOU with IIP, Dehradun, and CDAC-Bengaluru last semester.



Also, we have successfully conducted a two-day national conference on the "Advanced Materials for Environmental Sustainability-AMES 2023" conference from the 12th to 13th of Oct 2023 at MIT Manipal and organised guest lectures on diverse domains.

I am excited to share that our department is shifted to new premises in the Academic Block-2. This marked an important step in enriching research facilities and enabling teaching-learning with advanced technologies to improve our academic standards. We believe these initiatives will foster high-quality research and academic excellence in our department for the years to come.

Best regards,

Dr. M. Srinivas Kini Professor & Head, Department of Chemical Engineering Manipal Institute of Technology, MAHE, Manipal-576104. Email: srinivas.kini@manipal.edu

From the Students

ENERGY CONVERSION AND STORAGE IN POROUS MATERIALS

Santusti, Rishith (B.Tech. Batch of 2026) & Adyasha Kar (B.Tech. Batch of 2024)

In the rapid technological and industrial advancement era, the world grapples with pressing challenges: energy scarcity and environmental degradation. Over 80% of energy consumption relies on non-renewable fossil fuels, intensifying resource depletion and environmental decay. The resulting emissions of greenhouse and acidic gases further contribute to global climate deterioration. Addressing these issues necessitates practical and cost-effective solutions. Porous polymeric and carbonaceous materials emerge as promising contenders, featuring well-developed porosity and tuneable surface chemistry. Their functionalized pore structures enhance their suitability for environmental treatment and energy storage, making them pivotal components in diverse systems aiming for the physical/chemical confinement of substances within their walls and voids.



The complex xylem and phloem branching structure in plant leaves

Among the materials reviewed thus far, mesoporous, and macroporous materials are the most suitable for energy conversion/storage applications. Recent advances in the synthesis and fabrication of mesoporous and macroporous architected materials have proven to be diverse and specific to applications, even though broad-spectrum ones also are carried out—soft-templating methods that use supramolecular entities containing self-assembled arrays of structure-directing molecules such as surfactants. Soft molecules in soft-templating techniques may self-assemble into a broad range of ordered nanostructures; hence, this technology offers significant benefits in regulating method, where porous materials' porosity shape/size. Another process is the Hard-Templating method, where porous materials are developed from an interactive replication between a precursor and its template. Various 3D printing technologies, including Stereolithography (SLA), Direct Ink Writing (DIW), Fused Deposition Modelling (FDM), Selective Laser Melting (SLM), Laminated Object Manufacturing (LOM), Binder Jetting (BJ), and Inkjet Printing (IJP) have been used to fabricate energy conversion/storage devices. Porous materials' performance in energy storage and conversion devices, i.e., their ability to store and convert energy, is heavily influenced by their pore structure.

As a result, careful control of the size, shape, and distribution of pores in manufactured porous materials is critical.

Conjugated porous polymers are considered candidates for solar energy conversion due to their thermal and photochemical properties. Their application ranges from energy storage to energy conversion in metal-ion batteries, metal-air batteries, water splitting and fuel cells. Carbon spheres are porous hollow shells of carbon, ranging in size from millimetres to nanometers. They are reported to be superior to other carbon-based agents due to their high photothermal conversion efficiency of 54.2%. Thus, the high conversion efficiency of carbon spheres is crucial in photothermal therapy, where they convert near-infrared lasers into thermal energy to kill tumour cells.

Functional porous materials like polymeric and carbonaceous compounds show great promise in tackling global energy and environmental issues. With well-defined pores, they find applications in environmental treatment and energy storage. Challenges ahead include designing materials that balance surface area and functionality, optimising production processes for real-world use, and gaining deeper insights into how these materials work. Overcoming these challenges will lead to high-performance solutions. The current strategies set the stage for future advancements in creating more sustainable technologies to address the pressing concerns of energy scarcity and environmental impact.

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Revolutionizing Water Treatment: The Power of 3-D ZnO Structures in Sertraline Photocatalysis

Santusti, Rishith (B.Tech. Batch of 2026) & Aditya Gupta (B.Tech. Batch of 2024)

ZnO possesses photocatalytic properties and can generate reactive oxygen species (ROS) under UV light stimulation, making it an efficient photocatalyst. Researchers have been able to test this ability of ZnO to synthesize a hierarchal structure of 3-D ZnO, which degrades antidepressants that have been polluting our environment, the most prominent being water pollution. Since 3-dimensional structures retain more surface area than 1-dimensional and 2dimensional materials, they proved to be more efficient at breaking sertraline than existing methods and processes. Sertraline is a selective serotonin reuptake inhibitor that lowers blood glucose levels and is used to treat depression and improve glycemic control in diabetic patients. Because sertraline is a weakly soluble chemical, it can only be taken orally. Although its concentration is relatively low, concerns such as bioaccumulation and the effect on the nervous system have risen that cause effect to aquatic life.

The imposed limitations by the government and several health organizations around the world for the allowable levels of sertraline in wastewater discharge is 326 ng/L in the influent and 374 ng/L in the effluent of 19 wastewater plants around metropolitan areas in Europe, Asia, America, as well as Africa but the concentrations, exceed the limit to reach the numbers of around 641 ng/L which does not prove to be beneficial to the ecosystem. This is happening because of great human waste discharge, pharmaceutical industrial discharge, and the uncontrolled disposal of medical waste through incorrect methods by the population. Certain rules, regulations, and initiatives need to be put forth to reduce this.

The implications of having such high levels of sertraline in the water that is discharged into the ecosystem are that it affects the growth of aquatic life as well as plants by shortening their roots' length, which offers them lesser stability and a greater chance of being part of runoff, thus reducing the soil quality in the region as well; moreover, the bioaccumulation of it in the food chain affects multiple food webs and the quaternary consumers at the top suffer from changes to their bodies and organ functions.



The copious levels of Sertraline in the natural water bodies.

Hence there has been active research in discovering the optimum solution without harming the environment. An attempt to study the biotransformation of sertraline during its removal from wastewater revealed that it is only partially degradable. In the process of trying to eradicate this component's presence in the water through several methods, researchers have produced a few methods such as using gamma radiation, using different bacterial cultures in the normal sewage treatment process to try and breakdown the impurity. However, most of them have proven to be relatively inefficient to ZnO. ZnO was chosen because no prior investigation as an anti-depressant degradation photocatalyst had been done, as well as because of its low cost and easy to synthesize methods whose products also yield great efficiencies to further processes.

To test their photocatalytic ability, solutions in ultrapure water were made with each containing 5mg of different semiconductors obtained and 10 mg (which is about the weight of a grain of table salt) of sertraline [SRTL]. Before their photocatalytic assays, they were kept in a dark environment with continuous agitation to reach the adsorption-desorption equilibrium. The samples were then irradiated with UV light at 254 nm and 0.94 mWcm-2 in a photochemical reactor for 5 to 60 minutes.

Since Zn9 was able to show a comparatively greater output in each aspect, like adsorbing capability which was discovered using the Brunauer-Teller and Emmet Theory, reusability after five cycles as well as the time required for breakdown SRTL and RhB, it was selected for further use and applications; moreover, it was also the easiest to procure out all the tested samples. There are certain effects that occur over each cycle, the biggest one being a reduction in photocatalytic activity due to the poisoning of the photocatalytic surface, but that can be removed through washing and heat treatment.

This approach towards clearing contaminants out of wastewater has resulted in several beneficial findings, an efficient photocatalyst that is reusable after multiple cycles with minimal reduction in efficacy, remaining at 80% due to incredibly high stability. The experimental results confirm that the 3-dimensional Zinc-Oxide is an effective photocatalyst that is produced through high-control synthetic systems that manage to produce high performance in the breakdown of SRTL pollutants in natural waters.

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Department Events

Guest Lecture in Department of Chemical Engineering

Dr K Sudhakar a Faculty of Mechanical and Automotive Engineering Universiti Malaysia Pahang delivered four guest lectures:

- (1) "Carbon Capture, utilization and Storage for a Sustainable Future" on 08-08-2023.
- (2) "Green Hydrogen Status, Trend and Perspectives" on 08-08-2023.
- (3) "Sustainable Biofuels & Biochemicals from Bio residues & Waste Resources" on 09-08-2023.
- (4) "Phase Change Materials and Their Applications" on 09-08-2023.



MOU signed between MIT Manipal & Indian Institute of Petroleum Dehradun

Department of Chemical Engineering at MIT has taken a step forward to begin a new journey of transformative and ground-breaking research in the field of alternative energy to sign an MoU with CSIR, Indian Institute of Petroleum (IIP) Dehradun on 29th Aug 2023. The major scope of this MoU includes Joint Research Programs, Academic / Training-Related Programs such as Mutual guest lectures / seminars / workshops, internship opportunities for MAHE students in the area of clean energy. The MoU is largely going to focus on Sustainable Development Goal No. 7 of UNDP towards "Affordable and Clean Energy".

Commander (Dr.) Anil Rana, the Director of MIT, presided over the event. The Joint Director, Associate Directors, and Heads of various departments were in attendance. The gathering was warmly welcomed by Dr. K.V. Sriram, the Associate Director for Industry Liaison at Placement

& Practice School. Providing insights into the MoU, Dr. K. Balakrishna Prabhu, Professor & Head of the Department of Chemical Engineering, outlined its vast potential and opportunities. Dr. Anil Kumar Sinha, Senior Principal Scientist, Biofuels Division, IIP-Dehradun, engaged in insightful discussions with peers. Following this exchange, the MoU was formally signed.



Dr K Krishnaiah, Professor Emeritus, Former HOD, Dept of Chemical Engineering, IIT Madras, Chennai, Former Dean (Academics) IITM & IITT MAHE delivered the "MAHE-Class of 1994 Golden Jubilee Lecture" titled "Chemical Engineering in 21st Century" on 04-09-2023.





Schrodinger Material Science Workshop 4th - 6th September 2023

Schrödinger Material Science Workshop was organised from 04-Sep-2023 to 06-Sep-2023 by the Department of Chemical Engineering in association with the Dept. of Computer Science & Engineering at Manipal Institute of Technology, Manipal. Our esteemed Vice Chancellor Lt. Gen. (Dr.) M. D. Venkatesh had inaugurated the workshop and graced the occasion as the chief guest. The event was a grand success, with the Vice Chancellor's inspiring words profoundly impacting the audience to pursue interdisciplinary research as the way forward.

Computational molecular modelling is a powerful tool that can be used to understand and predict molecules' behavior and bridge the gap between different disciplines. The workshop featured introductory lectures on molecular simulations and hands-on training sessions about the applications in the fields of materials science, chemical engineering, chemistry, biology,

biotechnology, nanotechnology, physics, and engineering. The workshop introduced Molecular Modelling tools and demonstrated the capabilities of the Schrödinger Suite to participants with hands-on training sessions by Schrödinger Scientists. The audience comprises students, faculty members, and researchers from various institutes of MAHE participated enthusiastically.



A wide range of topics are covered in the workshop: (i) Catalysis and reactive Systems, (ii) Polymeric Materials, (iii) Energy Capture and Storage, (iv) Drug Discovery, (v) Metals, Alloys, and Ceramics. The field of computational molecular modelling is rapidly growing and evolving. Working towards interdisciplinary areas with applications in diverse fields is becoming increasingly important. Participants have gained the skillset and expertise to work with computational tools that assist them in staying ahead of the curve and solving real-world problems. Overall, the workshop provided essential ideas, motivation, and background about molecular simulations in material science.

Guest Lecture on "Systems Engineering Perspective of Human Physiology-Multiscale Models for Disease Characterization"



Prof K V Venkatesh from the Department of Chemical Engineering, IIT Bombay delivered a lecture on "Systems Engineering Perspective of Human Physiology-Multiscale Models for

Disease Characterization: Towards Drug Discovery, Clinical Study, Disease Management and Personalization" on 15th of September, 2023.





National Conference on "Advanced Materials for Environmental Sustainability-AMES-2023"

The Department of Chemical Engineering, MIT Manipal, organized a Two-day National Conference on "Advanced Materials for Environmental Sustainability-AMES-2023" on 12th and 13th of October 2023. The event was sponsored by ONGC-MRPL Ltd, BASF Ltd, and MCF Ltd. Mangaluru.

As a part of the event, technical paper presentations, poster presentations and invited guest talks were organized. More than thirty participants from both Manipal and other locations presented their technical papers or posters.

The AMES 2023 conference commenced with its inauguration function, led by Professor N.N. Sharma, the Pro-Vice-Chancellor Strategy and Planning of MAHE, who was the Chief Guest. The event was graced by Guests of Honour Dr. Nitin Labhsetwar, Chief Scientist at the National Environmental Engineering Research Institute (NEERI) Nagpur, and Mr. H.C. Sathyanaryana, GGM Technical Services at MRPL Mangalore. Professor Somashekara Bhat, Joint Director of MIT Manipal, presided over the function. Professor Balakrishna Prabhu, the Organizing Secretary and Head of the Chemical Engineering Department welcomed the gathering and Associate Professor Harshini Dasari, the Conference Convener proposed the vote of thanks.



During the event, the speakers emphasized the pivotal role of materials/nanomaterials, energy, and biofuels in environmental sustainability.

On the first day of the conference, Dr. Nithin Labhsetwar, Chief Scientist at NEERI, delivered the keynote address on the topic 'Low-cost materials for cleaner energy and environmental applications.' During his speech, Dr. Labhsetwar emphasized the crucial role of materials in the context of the environment and sustainability.

Mr. Vishnu Sharma, Director of Aapaavani Environmental Solutions, Mangalore, delivered the second guest talk titled "Exploring Nanotechnology for Environmental Sustainability." During his talk, Mr. Sharma emphasized the significance of recycling waste plastics and converting them into useful products. He also discussed the treatment of water and wastewater, highlighting their vital roles in environmental sustainability.

On the second day, two guest talks were conducted.

Dr. Ganapathi Ayappa delivered Prof PG Krishnamurthy memorial lecture titled 'Developing Adsorbed Natural Gas Solutions for Transport: From Molecules to Vehicle.' This lecture was

dedicated to the memory of Prof. P. G. Krishnamoorthy, who was a professor in the Chemical Engineering Department.



Dr Ayappa pointed out that the future of chemical engineering cannot be imagined without materials and their role in human life.



Mr T S Vishwanathan, Technical facilitator, Ion Exchange Ltd spoke on the topic "Membranes in water and wastewater treatment" emphasizing the role of membrane technology in water and wastewater treatment.

The distinguished speakers emphasized significant advancements in materials development related to sustainability, encompassing energy, environment, and water-related innovations.

The valedictory function on the second day featured Prof. K. Ganapathy Ayappa, Professor in the Department of Chemical Engineering at IISc, Bangalore as chief guest, and Mr. Harihara J, JGM-EHS and QC at MCF Ltd. Mangalore as the Guest of Honour. Cdr. Dr. Anil Rana, Director of MIT Manipal presided over the function. Organizing Secretary and Head of the Chemical Engineering Department, Prof. Balakrishna Prabhu welcomed the gathering and Conference co-convener Prof. S V S R Krishna Bandaru proposed the vote of thanks. Participants shared their personal experiences of the conference, expressing sincere gratitude for the opportunities provided. Finally, the distribution of certificates to the participants was conducted by the dignitaries.



MAHE MoU with CDAC to access Super Computer - Param Utkarsh

MAHE has signed an MoU agreement with CDAC Bengaluru to provide access to High Performance Computing facility. CDAC also facilitates the high-performance computing environment to work on multiple niche domains such as parallel programming, quantum computing, molecular simulations, IoT, artificial intelligence, machine learning, cybersecurity, CFD, GPU programming, Semantic mining, BIG Data, IPR, and Technology Management. Param Utkarsh is a supercomputer at CDAC Bengaluru. All users from MAHE can access the Param Utkarsh facility and work on the HPC environment. Many events and hands-on sessions for computational tools, are planned to train and upskill the workforce at MAHE. All MAHE campuses across India can benefit from this facility. Faculty/students/researchers concerned with using/requiring access to HPC are requested to contact Dr Srikanth Divi (srikanth.divi@manipal.edu).



Faculty Achievements



Dr. Harish Kumar S, Professor, Department of Chemical Engineering, Manipal Institute of Technology (MIT), Manipal, assumed the position of **Director – Corporate Relations**, **MAHE**, **Manipal**, effective July 01, 2023.

Grants Awarded to Faculty



Dr. Nethaji S., Department of Chemical Engineering (MIT, Manipal), in collaboration with Dr. Kapil Sadani, Instrumentation & Control Engineering (MIT, Manipal), Dr. Pooja Nag, Mechatronics Engineering (MIT, Manipal) and Chiranjay Mukhopadhyay, Manipal Institute of Virology, Manipal have received a grant on *"Technologies for screening and remediation of colistin and doxycycline from hospital effluents"* from Indian Council of Medical Research (ICMR) of rupees 1,43,91,556.60/- in 2023 for 3 years.

Student Achievements



Akshatha Hebbar and Devangshi Debraj (Batch of 2023) have received B.Tech. Honors degree in Chemical Engineering at Convocation-2023 conducted during November, 2023 at MAHE, Manipal.



Journal Publications

By Faculty & Students (From January 2023 to December 2023)

- 1. Ponnurangam, M., & Balaji, S. (2023). Tune in to the terrific applications of turanose. European Food Research and Technology. https://doi.org/10.1007/s00217-023-04417-4
- Debraj, D., Carpenter, J., & Vatti, A. K. (2023). Understanding the Effect of the Oil-to-Surfactant Ratio on Eugenol Oil-in-Water Nanoemulsions Using Experimental and Molecular Dynamics Investigations. Industrial & Engineering Chemistry Research, 62(41), 16766-16776. https://doi.org/10.1021/acs.iecr.3c02345
- 3. Debraj, D. and Lavanya, M., 2023. Microplastics everywhere: A review on existing methods of extraction. Science of The Total Environment, p.164878.
- 4. Somashekara, D. and Mulky, L., 2023. Sequestration of contaminants from wastewater: a review of adsorption processes. ChemBioEng Reviews, 10(4), pp.491-509.
- 5. Rao, P. and Mulky, L., 2023. Erosion-Corrosion of Materials in Industrial Equipment: A Review. ChemElectroChem, 10(16), p.e202300152."
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- Vinayagam, R., Hebbar, A., Kumar, P. S., Rangasamy, G., Varadavenkatesan, T., Murugesan, G., ... & Selvaraj, R. (2023). Green synthesized cobalt oxide nanoparticles with photocatalytic activity towards dye removal. Environmental Research, 216, 114766. https://doi.org/10.1016/j.envres.2022.114766
- Vinayagam, R., Quadras, M., Varadavenkatesan, T., Debraj, D., Goveas, L. C., Samanth, A., ... & Selvaraj, R. (2023). Magnetic activated carbon synthesized using rubber fig tree leaves for adsorptive removal of tetracycline from aqueous solutions. Environmental Research, 216, 114775. https://doi.org/10.1016/j.envres.2022.114775
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Conference Proceedings

- J. Carpenter, A. B. Pandit. Ultrasonication assisted Oil in Water emulsification: Some insights into the lipid oxidation stability of Emulsion. In 5th Asia-Oceania Sonochemical Society International Conference (AOSS-5), NIT Warangal, 28 to 30th September 2023.
- Anoop. K. Vatti, J. Carpenter. Understanding the effect of oil to surfactant ratio on eugenol oil in water nanoemulsion using combined experiments and molecular dynamics simulations. In 5th Asia-Oceania Sonochemical Society International Conference (AOSS-5), NIT Warangal, 28 to 30th September 2023.
- Ramyashree MS, Anirudh K.S, S.Shanmuga Priya Photocatalytic reduction of carbon dioxide using ZIF-8@BiVO4/rGO nanocomposite INCEEE 2023, Warangal Andhra Pradesh, 24th - 25th Nov 2023.
- Ramyashree MS, S.Shanmuga Priya, Veekshit Udayakumar Ail Synthesis and characterization of TiO2-Cu3(BTC)2 metal organic framework based advanced materials for photocatalytic CO2 reduction, RAMMML 2023, Nagpur, Maharashtra, 2nd – 4th Feb 2023".

Invited Talks

- Dr. Jitendra Carpenter delivered an Invited Early Career Research Lecture on "Ultrasonication assisted Oil in Water emulsification: Some insights into the lipid oxidation stability of emulsion" at the 5th Asia-Oceania Sonochemical Society International Conference (AOSS-5), NIT Warangal, 28 to 30th September 2023.
- Dr. Anoop Kishore Vatti delivered an Invited Early Career Research Lecture on "Understanding the Effect of Oil to Surfactant Ratio on Eugenol Oil in Water Nano-emulsion using Combined Experiments and Molecular Dynamics Simulations" at the 5th Asia-Oceania Sonochemical Society International Conference (AOSS-5), NIT Warangal, 28 to 30th September 2023.

Fun Zone

CROSS WORD PUZZLE Rishith Rajesh Khanna (Batch of 2026)



Down:-

Vertical :

1. When a process proceeds in such a manner that the system always remains practically in equilibrium.

2. I am not a scientist, but I have a degree in weather and ovens. What am I?

4. This process adds water vapor to the air without varying the temperature and proves to be quite useful in desalination methods.

5. The process of combining alcohols and acids, only to form a fruity and sweet-smelling product that is added to various food as flavourings and as well as a key ingredient in perfumes.

6. When the absolute pressure is zero atmospheres, I exist.

9. The number of particles, when equivalent to Avogadro's number, is present in one of me. What am I?

11. I am not a kilowatt-hour nor a foot-pound, But in energy units, I am quite renowned. What am I?

13. When my Latin name is translated to modern-day English, it reads as "Royal Water" and when freshly prepared, I am colourless but within a few seconds I go from yellow to orange to red. What am I?

Across:-

3. Fortunately, I am lucky to be unique by my name because it is the only one to begin with a "Y" out of all the elements that have been discovered till date.

7. Everyone use this chart to determine various data with regards to moist air, my X-axis is that of temperature and my Y-axis is of Humidity.

8. I am not a barometer but when measuring pressure, I am as handy as can be, especially when it comes to fluids, I am a regular performer. What am I ?

10. Named after the first person who won two Nobel prizes and discovered the elements which were used to make 'glow in the dark' watch dials as well as treat cancer, I am one of the units used to measure radiation.

12. This type of flow has a relatively smaller range when it comes to Reynold's number.

14. I am used to speed up the Ostwald Process and am among the rare elements on this planet. What am I ?

15. This operation is used to remove water at relatively lower temperatures in smaller quantities using a carrier gas so as to get solids from wet substances.

16. This method is used to remove any unwanted components from the Recycle stream of an operation or process where the unconverted reactants in the products are fed back to the start.

CROSS WORD PUZZLE ANSWERS

Purge	.8
Drying	.T
Platinum	.9
sipaЯ supA	·S
WolA noitianaT	·4.
əluoc	3.
Curie	5.
aloM	·L

.8	Manometer
.Γ	Psychrometric
.9	munoeV
.5	Esterification
4 .	Humidification
3.	Mutrium
2.	Fahrenheit
٦.	Quasistatic

Alumni Reminiscences

Here comes a fantastic opportunity for our MIT alumni. Pen down your best memories, thoughts, lessons, and experiences you have had on our campus in your college days and get them published in our next Tempus issue! Hoping to read the mind-boggling stories and epic pictures



https://forms.office.com/r/rS8rY7SWf3

TEMPUS Archives

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