DST-SERB Sponsored Third International Conference on Functional Materials for NextGen Applications

ICFMNA`25

3rd and 4th February 2025

Organized by

Department of Chemistry
Sri Sivasubramaniya Nadar College of Engineering,
Kalavakkam – 603 110

In Association with

THE SOCIETY FOR POLYMER SCIENCE, INDIA
CHENNAI CHAPTER

Prof. S. Radha
Principal, SSN Institutions

I am immensely pleased to announce that the SSN Institutions, in association with the Society for Polymer Science (Chennai Chapter), is organizing the **DST-SERB Sponsored Third International Conference on Functional Materials for Next-Gen Applications (ICFMNA 2025) from 3rd to 4th February 2025**. This prestigious conference will feature six distinguished international keynote speakers from **West University of Timisoara, Romania**, and one expert from **Nagoya University, Japan**, along with five esteemed speakers from renowned Indian labs including **CSIR-CSMCRI, C-MET, VIT, Pondicherry University, and Shiv Nadar University.**

I am delighted to recall the success of previous conferences that brought together leading researchers and provided a platform for fruitful discussions. The **ICFMNA 2025** promises to continue this legacy, providing valuable insights into the latest advancements in functional materials and their applications. The event will foster international collaboration and provide an excellent opportunity for scientists, academicians, and researchers to share ideas and explore cutting-edge technologies.

The presence of renowned speakers from institutions such as West University of Timisoara, Nagoya University, and leading Indian research labs will be a source of great motivation for attendees, further strengthening the bridge between global scientific communities. I am confident that this conference will inspire young researchers and create new avenues for interdisciplinary research, paving the way for innovations that will benefit society.

I extend my heartfelt congratulations to the conference conveners, organizing committee, and all those involved in making **ICFMNA 2025** a reality. I am certain that all delegates will find the program immensely enriching and engaging.

I wish the conference great success and look forward to the inspiring discussions that will take place during this landmark event.

Prof. S. Radha

Prof. P. Ramasamy
Dean (Research), SSN Institution

I am happy that Department of Chemistry, SSN Institutions, in association with the **Society for Polymer Science of India (Chennai Chapter),** is organizing the **DST-SERB Sponsored Third International Conference on Functional Materials for Next-Gen Applications (ICFMNA 2025) on 3rd and 4th February 2025**. The conference will feature active participation and insightful discussions among leading researchers, including prominent international keynote speakers from **West University of Timisoara, Romania, Nagoya University, Japan**, and top Indian labs such as **CSIR-CSMCRI, C-MET, VIT, Pondicherry University, and Shiv Nadar University.** I am confident that the eminent resource persons, with their wide experience in functional materials and next-gen applications, will provide a new impetus to budding researchers, giving them a strong platform for the exchange of ideas and fostering international collaborations.

To be a successful researcher, one must continually update their knowledge with the latest developments in their chosen field. This requires active participation in serious scientific conferences. Physical participation in such events creates lasting connections, impressions, and bonds of friendship and networking, which can prove invaluable over time. I understand that **ICFMNA 2025** will feature keynote talks from renowned experts, along with over 150 authors presenting papers. Organizing a conference of this scale is a major undertaking, but I am confident that the extensive experience of the organizing committee will ensure the success of this event.

I extend my heartfelt congratulations to the conference conveners and the organizing committee of **ICFMNA 2025** for their dedicated efforts in making this event a reality. I wish **ICFMNA 2025** a grand success, and I am certain that all delegates will find the program immensely enriching and impactful. I would also like to acknowledge the strong support provided by the management of SSN Institutions, whose backing has been crucial in bringing this important international event to life for the Materials Science community.

Prof. P. Ramasamy

Professor S. Sivaram, FNA

IISER Pune

I am very happy to note that the Department of Chemistry, SSN College of Engineering is organizing an International Conference on Functional Materials for NextGen Applications (ICFNA 2025) in association with The Society for Polymer Science (SPS-I), Chennai Chapter on 3-4 February 2025 at its Kalavakkam, Chennai Campus. This Conference aims to bring international researchers, academicians and industrialists under one roof to discuss various advancements in the field of functional materials for future applications. Functional materials constitute an interdisciplinary subject requiring participation from all branches of chemical, physical, biological sciences as well as related disciplines of engineering and technology.

The Conference is, both, timely and relevant. Functional materials are key to major challenges in human health, built habitats, environment and energy, which together, constitute the important pillars of the global sustainability agenda. Several important problems are crying for urgent solutions and, if solved, will have large social and economic impact. Research must, therefore, focus on what "needs to be done" rather than "what can be done". It must address the complexity inherent in such problems which can be solved only by cross disciplinary teams. Our higher educational institutions must break the narrow discipline-oriented silos in which they generally work and forge collaborations, both within and outside the institutions. I hope that this Conference, which has substantial international participation, will set aside some time to deliberate these emerging challenges and how the scientific community can respond to them.

I wish the Conference a grand success.

S. Sivaram

Prof. S. SIVARAM

Prof.Dr. E. Murugan., Ph.D., FRSC., FASch.,
Dean-Research
Professor & Head
Department Of Physical Chemistry
University of Madras
President – SPSI (Chennai Chapter)

From the onset, I am truly happy to know that the Department of Chemistry, SSN College of Engineering, Chennai is proudly organizing its **Third International Conference on "Functional Materials for NextGen Applications – ICFMNA`25" during 3rd and 4th February 2025.**

Being in a higher education fraternity, I have long held an opinion that the vibrant atmosphere of the college has always had ambitions of providing students high academic achievements. SSN College of Engineering being a Key unit of the SSN Institutions, is not only serving well towards the engineering and Technological community but also has Profusely contributed to the development of Science and Humanities. This Central unit among the Institutions was established in 1996 affiliated to Anna University aiming to foster intellectual growth, free-thinking, and personal development by offering dynamic learning opportunities that prepare students with the skills, insights, and experiences necessary to contribute responsibility to society. I understand that this institute is currently accredited with A^{++} grade by NAAC, within 22 years has emerged as one of the leading educational institutions in the country and has achieved autonomous status in 2018.

As a Chemical Science Fraternity at the University of Madras as well as the President of SPSI Chennai Chapter I have had an opportunity to interact with the Department of Chemistry. The Department has a solid foundation for Applied chemistry, which is vital for all engineering branches. However, for inculcating high standards of Scientific skills and research on significant social technologies, a distinct Chemical Science Research Centre has been established. An International Conference of this kind shows the commitment to fostering innovation, promoting groundbreaking research, in the field of materials science by the Department. Through such endeavors, the department proves to provide a quality research experience to the young research Scholars and budding scientists of the Scientific Community. Conferences like this serve as vital platforms to emphasize the significance of polymers, nurturing collaboration, sharing innovative ideas, and showcasing the latest advancements in polymer science. I firmly believe that this conference would undoubtedly widen the horizons in Chemistry by exchange of ideas and fruitful interactions among the potential researchers.

I sincerely applaud the organizing committee for making an effort to uncover the beauty lying in various arena of chemistry within two days in this ICFMNA`25. To the Management, Principal Prof.

V. E. Annamalai, Conference Chair and Head, Department of Chemistry Dr. M. Siluvai Michael, Convenors Dr. A. Murugesan, Dr. S. I. Davis Presley, Dr. N. Priyadarshini, the Organizing Committee and their team, I extend my warmest regards and best wishes for the tremendous success of the conference.

Prof. Dr. E. MURUGAN

Dr. S. N. Jaisankar
Secretary, SPSI (Chennai Chapter)
Former Chief Scientist, CSIR-CLRI, Chennai

Dear R & D community of the Materials Industry

It is a great pleasure and honour to extend you a warm invitation to attend the I**nternational Conference on Functional Materials for Next-Gen Applications 2025 (ICFMNA'25)** to be held at Chennai, India for the third time at Sri Sivasubramaniya Nadar (SSN) College of Engineering, Tamil Nadu, between February 3 and 4, 2025 in association with the **Society for Polymer Science** (Chennai Chapter), ICFMNA'25. The conference promises to be a special one on account of the quality and type of participation and the vastness of the nature of topics planned to be discussed in the Science and Technology of functional materials. The conference has several invited speakers, oral and poster presentations that will be presented by eminent academicians, researchers and students worldwide. We will have a very interesting discussion on important and relevant issues concerning the global materials energy sector. With many innovative things planned, this conference will raise the bar for future materials. As a secretary of the SPSI, Chennai chapter and advisory committee member of the conference, I know that the success of the conference depends ultimately on many people who worked with us in planning and organizing both the technical program and supporting social arrangements. Recognition should go to the local organizing committee members who have all worked extremely hard for the details of important aspects of the conference programs. We hope you will join us for a symphony of outstanding science and take a little extra time to enjoy the spectacular and unique beauty of the region. Thank you and best regards to all

Dr. S. N. JAISANKAR

Dr. A. Murugesan
Convenor, ICFMNA 2025
SSN Institution, Kalavakkam

The main objective of the **DST-SERB Sponsored 3rd International Conference on Functional Materials for Next-Gen Applications (ICFMNA 2025)** is to bring together eminent researchers from across the globe to share their ideas and recent developments in the field of functional materials, nanoscience, and advanced technologies. I would like to extend my heartfelt thanks to the Scientific and Technical Committee for their untiring support in organizing this important international event. I also convey my sincere appreciation to the **Society for Polymer Science (Chennai Chapter)** and all our partners for their valuable contribution to this conference.

ICFMNA 2025 received around 150 high-quality submissions, with the most impactful research selected for presentation. We thank our international reviewers and steering committee for their efforts. The selected papers will be presented in various formats by experts from India and abroad, covering materials science, functional materials for bio and energy applications, and next-gen technologies.

I would like to place on record my thanks to the distinguished keynote speakers and many others. I extend my sincerest congratulations to all authors and speakers for their valuable contributions. I would also like to express my deepest gratitude to the Chief Patron, **Dr. Shiv Nadar**, Founder of SSN Institutions and Chairman of HCL Technologies, the Patron, **Dr. Kala Vijayakumar**, President of SSN Institutions, **Dr. S. Radha**, Principal of SSN College of Engineering, **Prof. P. Ramasamy,** Dean of Research at SSN Institutions and all the faculty members of SSN Institutions who have been instrumental in making this international conference a reality.

Lastly, a special thank you goes to our students and research scholars who have gone above and beyond in supporting the organization of this event. Their dedication and hard work have been vital in ensuring the smooth execution of this conference.

Dr. S.I. Davis Presley
Convenor, ICFMNA 2025
SSN Institution, Kalavakkam

The primary aim of the **DST-SERB Sponsored 3rd International Conference on Functional Materials for Next-Gen Applications (ICFMNA 2025)** is to gather distinguished researchers from around the world to exchange ideas and present the latest advancements in functional materials, nanoscience, and emerging technologies. I would like to express my sincere gratitude to the Scientific and Technical Committee for their unwavering support in organizing this significant global event. My heartfelt thanks also go to the **Society for Polymer Science** (Chennai Chapter) and all our partners for their valuable contributions to the success of this conference.

We thank our international reviewers and steering committee for their efforts in curating the outstanding contributions to **ICFMNA 2025**. Selected papers will be presented in various formats by esteemed experts from India and abroad, covering materials science, bio and energy applications, and next-gen technologies. Special thanks to our distinguished keynote speakers, including experts from **West University of Timisoara, Nagoya University, and leading Indian institutions**. We appreciate the contributions of all authors and speakers and believe the discussions will advance knowledge in these fields.

My deepest gratitude goes to our **Chief Patron, Dr. Shiv Nadar, Patron, Dr. Kala Vijayakumar,** and the SSN leadership for their crucial role in organizing this event. Lastly, a special thank you to our students and research scholars for their hard work in making this conference a success. We are confident that the academic discussions will inspire innovative ideas throughout this two-day event.

Dr. N. Priyadarshini
Convenor, ICFMNA 2025
SSN Institution, Kalavakkam

The main aim of the **DST-SERB Sponsored 3rd International Conference on Functional Materials for Next-Gen Applications (ICFMNA 2025)** is to bring together distinguished researchers from across the globe to share their insights and showcase the latest breakthroughs in functional materials, nanoscience, and emerging technologies. I would like to sincerely thank the Scientific and Technical Committee for their tireless work in organizing this prestigious international event. My gratitude also extends to the **Society for Polymer Science (Chennai Chapter)** and all our collaborators for their invaluable support in making this conference a success.

I would like to place on record my thanks to the distinguished **keynote speakers** and many others. I extend my sincerest congratulations to all authors and speakers for their valuable contributions. I would also like to express my deepest gratitude to the Chief Patron, **Dr. Shiv Nadar**, Founder of SSN Institutions and Chairman of HCL Technologies, the Patron, **Dr. Kala Vijayakumar**, President of SSN Institutions, **Dr. S. Radha**, Principal of SSN College of Engineering, **Prof. P. Ramasamy,** Dean of Research at SSN Institutions and all the faculty members of SSN Institutions who have been instrumental in making this international conference a reality.

Lastly, a special thank you goes to our students and research scholars who have gone above and beyond in supporting the organization of this event. Their dedication and hard work have been vital in ensuring the smooth execution of this conference. We are sure that all the distinguished invitees, delegates and scholars will benefit from the academic deliberations with tremendous ideas and visions during this two-days international conference

DST-SERB Sponsored 3rd International Conference on Functional Materials for NextGen Applications ICFMNA-25,

3rd and 4th February 2025 - Chennai, India.

Programme Schedule

Day - 1 (03.02.2025)

Venue: Justice Pratap Singh (Main) Auditorium, SSN Institutions

Registration: 8.30 am to 9.30 am

Inauguration: 9.45 am to10.45 am

Tea break : 10.45 am to 11.00 am

Talk	Time	Speakers name	Institution
Session Chair: Dr. Tanusree Sengupta, SSNCE, Chennai.			
Plenary talk-1	11.00 am to 11.40 am	**Prof. Daniel Vizman**	West University of Timisoara, Romania.
Session Chair: Dr. P. Prabhu, Univesity of Madras, Chennai and Dr. V.Tamilmani, SSNCE, Chennai.			
Keynote talk-1	11.40 am to 12.10 pm	**Prof. Bimlesh Lochab**	Shiv Nadar (Institution of Eminence) University, India.
Keynote talk-2	12.10 pm to 12.40 pm	**Prof. Stef Marius**	West University of Timisoara, Romania.
LUNCH-12.40 pm to 1.30 pm			
Oral Session-I	**Parallel Session 1.30 pm to 3.00 pm (Venue: Main Auditorium)**	**Session Chair: Dr. A. Muthukrishnaraj, Amrita Vishwa Vidyapeetham, Coimbatore and Dr. A.M.Shanmugharaj, SSNCE, Chennai.**	
		OP1 to OP10	
	Parallel Session 1.30 pm to 3.00 pm (Venue: Central Seminar Hall, ECE Annexure)	**Session Chair: Dr. K. Jayamoorthy, St Joseph's College of Engineering, Chennai and A. Chandrasekar, SSNCE, Chennai.**	
		OP11 to OP25	
Tea break: 3.00 pm to 3.15 pm			
Session Chair: Dr. S. Suresh, SRMIST, Chennai and Dr. N. Priyadarshini, SSNCE, Chennai.			
Keynote talk-3	3.15 pm to 3.45 pm	**Prof. Poienar Maria**	West University of Timisoara, Romania.

Invited talk-1	3.45 pm to 4.05 pm	**Dr. K. Rajendra Kumar**	Vellore Institute of Technology Chennai, India.
Poster Session – I	4.15 pm to 5.30 pm **(Venue: Main Auditorium)**	**Session Chair: Dr. T. Prakash, University of Madras, Chennai and Dr. S. C. Gurumurthy, Manipal Institute of Technology, Manipal**	
		PP1 to PP 45	
Oral Session- II	4.15 pm to 5.30 pm **(Venue: Main Auditorium)**	**Session Chair: Dr. S. S. Kalaivani, Amrita Vishwa Vidyapeetham, Coimbatore and Dr. A. Murugesan, SSNCE, Chennai**	
		OP 26 to OP34	
Cultural Programme	6.00 pm to 7.30 pm		

Day - 2 (04.02.2025)

Venue: Central Seminar Hall (Annexture) ECE, SSN Institutions

Talk	Time	Speakers name	Institution
Session Chair: Dr. S. C. Gurumurthy, Manipal Institute of Technology, Manipal and Dr. M. Siluvai Michael, SSNCE, Chennai.			
Plenary talk-2	09.00 am to 9.40 am	**Prof. Octavian Madalin Bunoiu**	West University of Timisoara, Romania.
Keynote talk-4	9.40 am to 10.10 am	**Prof. Gabriel Bușe**	West University of Timisoara, Romania.
Invited talk-2	10.10 am to 10.30 am	**Dr. Ketan Patel**	CSIR-CSMCRI, Bhavnagar, Gujarat. India.
Tea Break	**10.30 am to 10.45 am**		
Oral Session – III	10.45 am to 11.35 am **Venue: Central Seminar Hall, (ECE Annexure)**	**Session Chair: Dr. P.Panneerselvam SRM, Kattankulathur, Chennai and Dr. Davis Presley, SSNCE, Chennai**	
		OP35 to OP41	
Poster Session - II	10.45 am to 11.35 am **Venue: Central Seminar Hall, (ECE Annexure)**	**Session Chair: Dr. P. Rajkumar, Government Arts college for women Dindigul and Dr. M. Srinivasan, SSNRC, Chennai**	
		PP46 TO PP92	
Session Chair: Dr. M. Surendiran, AVIT, Chennai and Dr. T.Arun Luiz, SSNCE, Chennai			

Keynote talk-5	11.35 am to 12.05 pm	**Prof. Kutsukake kentaro**	Nagoya University, Japan.
Invited talk-3	12.05 pm to12.25 pm	**Dr. S. C. Gurumurthy**	Manipal Institute of Technology, Manipal.
Invited talk-4	12.25 pm to 12.45 pm	**Dr. P. Senthil kumar**	Pondicherry University, India.
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Invited talk-6	2.50 pm to 3.10 pm	**Dr. Madhav Ranganathan**	IITK, Kanpur, India.
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PL-01

Numerical simulation of unsteady thermal and oxygen transport in a Czochralski process for solar silicon growth

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Abstract

Nowadays Si-wafer based PV technology accounted for more than 95% of the total production in 2021. The market share of mono-crystalline technology is about 84% of total c-Si production. In order to meet the low-cost manufacturing criterion the Czochralski (CZ) crystal growth method which is the dominant technology for growing high quality monocrystalline silicon should be optimized. Defects and impurities incorporated in grown crystals during the growth process at the solid-liquid interface limits the efficiency potential of the grown crystals because they reduce the minority carrier lifetime. The solar cell efficiencies achieved by the different techniques correlate directly with the material quality, i.e. higher efficiency is achieved the less crystal defects and impurities are present in the material. Therefore, in order to increase the efficiency, a deep understanding of the underlying chemo-physical phenomena occurring during the crystallization process and their influence on the material properties is of utmost importance. Melt convection is acknowledged to be a very important factor in the field of crystal growth: Convective flows contribute to heat transfer and thus control the rate of solidification; The resulting temperature field in the vicinity of the solid-liquid interface affects its shape and therefore the generation of thermal stress and the formation of dislocations; Convection controls the species/impurity transport in the melt; It affects the dissolution rate of crucible materials, It affects the formation and transport of particles in the melt; Furthermore, in a complex interaction of both heat and species transport, convection strongly influences the morphology and stability of the solid-liquid interface. In a Cz process, time-fluctuations in temperature and in the concentration of impurities are mainly due to the melt convection with its two components: the natural convection and the forced convection generated by the rotation of the crystal and the crucible. In this contribution a numerical study using STHAMAS 3D software of the influence of different growth parameters (crucible and crystal rotations, pull rate) on the temperature and oxygen distribution will be presented for a 200mm Cz-configuration in order to show the role numerical methods can play in optimization of crystal growth process.

PL-02

Composite Materials Based on Magnetorheological Suspensions, Silicone Rubber and Polymeric Microfibres – Fabrication, Properties and Applications

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Abstract

Recently the scientific community has shown great interest in exploring new classes of advanced materials. This category includes composite materials based on magnetorheological suspensions, silicone rubber, microfibers from natural and artificial polymers, linear and non-linear dielectric microparticles and nano graphenes. Following this research direction, this paper aims to review methods for the production of such composite materials, their characterization methods, and the determination of their physical properties (electrical conductivity, magneto-rheological effects, stress and deformation fields, viscous elastic and strain coefficients) [1-8].

The produced materials are studied in a static magnetic field [1-8] over which a low and medium frequency electric field is superimposed [3,4,6]. Their thermal stability is also studied. Particle-to-particle interactions and elastic matrix in composites based on silicone rubber and nano-micro magnetizable particles are studied using the small-angle neutron scattering method [2]. The determined properties are useful for the purpose of manufacturing mechanical strain and stress sensors, electromagnetic wave and X-ray absorbers [8], tactile sensors and components for detecting electromagnetic fields, which are useful for patients with cardiac pacemakers [1,2,5,7,8].

The mentioned applications are described in detail, specifying their technical characteristics, while the physical mechanisms and theoretical models that determine and describe the properties of the involved materials, such as: magnetorheological materials, silicone rubber, natural and artificial polymer microfibers, linear and non-linear dielectric microparticles and nano-graphenes, are also presented.

Keywords: composite materials; magnetorheological materials.

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KT-01

Sustainable polymers: Waste- and bio-feedstocks are goldmines for innovative applications

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Abstract

Depleting fossil fuel reserves and increasing waste reservoirs are among the world's most pressing problems. This calls for exploring naturally occurring building blocks for developing bio-based polymers. Polybenzoxazine is a new class of thermally curable thermosets being pitched as superior alternates of phenolics. In this work, I intend to exploit the options of synthesizing partially bio-based polybenzoxazines following green chemical principles of atom economy, bio-renewable feedstock, solventless synthesis, and nontoxic waste generation. In addition, the molecular flexibility of benzoxazine moiety has been utilized by studying the relation between higher functionality and properties. These polymers have shown improved thermal stability compared to their non-green counterparts and the ability to copolymerize with elemental sulfur as one of the high-tonnage industrial wastes, thus finding wide applicability [1-5] from adhesive, antibacterial, water purification materials to cathodes for next-generation beyond Lithium-ion battery (LIB) and self-healing materials.

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KT-02

Growth and characterization of TmF_3 -doped fluorite crystals

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Abstract

Rare-earth-doped fluorite crystals have attracted considerable interest due to their exceptional optical properties and potential applications in various domains, particularly laser technology. Among these materials, CaF_2 or BaF_2 crystals doped with TmF_3 exhibit remarkable versatility in luminescent characteristics, making them highly promising candidates for advanced optical applications. This study investigates the luminescence of Tm^{3+} and Tm^{2+} ions in fluorite crystals synthesized in the Crystal Growth Laboratory using the vertical Bridgman method. A comprehensive Judd–Ofelt analysis was performed on Tm^{3+}-doped crystals to elucidate their spectroscopic properties and explore their application potential. The Judd–Ofelt theory offers a robust framework for examining optical transitions and calculating spectroscopic parameters of rare-earth ions embedded in crystalline hosts. For Tm^{3+} ions in the investigated crystals, the intensity parameters (Ω_2, Ω_4, and Ω_6) were determined, providing critical insights into radiative properties such as emission cross-sections, branching ratios, and quantum efficiencies, which are essential for designing advanced laser and optical systems. Recent progress in spectroscopic techniques and theoretical models has significantly enhanced the understanding of complex energy transfer processes and relaxation dynamics in Tm^{3+}-doped fluorite hosts. By integrating these advancements into the Judd–Ofelt analysis, this research offers a deeper understanding of the luminescence mechanisms and spectral features of Tm^{3+} ions, contributing to their optimization for laser applications

Acknowledgments

This work was supported by ESCARGOT project founded by the Romania's recovery and resilience plan, PNRR/2022/C9/MCID/i8.

KT-03

Influence of Rare-Earth doping on the morphology and crystal structure of fluoride MF_2 (M=Ca, Ba) single crystals

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Abstract

In the last years, trivalent Rare-Earth (RE^{3+}) ions doped fluoride MF_2 (with M = Ca or Ba) materials have been extensively studied due to the possibility to be used in various applications. The CaF_2 and BaF_2 fluoride materials crystallize into a cubic structure within the Fm-3m space group, characterized by Ba^{2+} or Ca^{2+} cations surrounded by eight F^- ions, while F^- atoms are enclosed by four Ba^{2+} or Ca^{2+} ions. The Re^{3+} doping into the host lattice is made without change in the symmetry and the excess of charge is compensated by interstitial F^- ions leading to different isolated site symmetry centers depending on the RE^{3+} concentrations i.e. at low RE^{3+}: tetragonal (C_{4v}), trigonal (C_{3v}) or cubic (O_h) or more or less complex clusters for higher RE^{3+} doping. The crystal structure of RE^{3+}= Er, Tm doped fluoride MF_2 (with M = Ca or Ba) materials, obtained by vertical Bridgman technique, has been analyzed by using X-Ray (laboratory and synchrotron) and neutron diffraction in order to provide more information about the changes induced by adding the RE^{3+} ions at various concentrations in the matrix. Moreover, spectroscopic investigations have been undertaken at room temperature in order to understand the complex relationships between the optical properties and the characteristics of fluoride doped crystal structure. In order to assess the optical quality of the obtained doped crystals, the dislocation density and the etch pits morphology has been evaluated and will be presented.

KT-04

Double doped Rare-Earth (RE=Er and Yb) CaF_2 and BaF_2 single crystals: synthesis and investigations of physical properties

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Abstract

Rare-earth (Er, Yb, Tm etc.) ions-doped calcium fluoride (CaF_2, BaF_2) crystals have been investigated due to the possible use in various applications. Among the rare earths, erbium-ytterbium doped fluoride matrix have potential to be used in fiber lasers, fiber amplifiers, and in diode-pumped bulk lasers. Fluorides crystalline matrix (CaF_2, BaF_2) is formed into a fluorite cubic structure (Fm-3m space group), with the fluoride cations surrounded by eight F^- ions, while F- atoms are enclosed by four Ca/Ba $^{2+}$ ions. The RE^{3+} (RE=Er, Yb) doping into the host lattice is made without change in the symmetry and the excess of charge is compensated by interstitial F- ions in different positions leading to isolated site symmetry centers at low content like tetragonal (C4v), trigonal (C3v), cubic (Oh) or more complex clusters for higher doping. These differences in site symmetries influence the optical characteristics. Different concentrations of Er^{3+}/Yb^{3+}-doped fluoride (CaF_2, BaF_2) crystals where grown by using an in-house vertical Bridgman configuration[4]. The study of the dislocations density using the chemical etching method was performed in order to characterize the crystal quality. Temperature and frequency dependence of the real and the imaginary part of the complex dielectric constant for ErF_3/YbF_3-doped fluoride crystals were studied. Optical investigations by absorption and emission spectroscopy were carried out at room temperature in order to point out the influence of Er and Yb content. Moreover, Judd–Ofelt (J–O) analysis was used to estimate the transition probabilities of Er^{3+} ion.

KT-05

Application of Machine Learning in the field of Applied Physics

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Abstract

As symbolized by the awarding of the 2024 Nobel Prize in Physics to Dr. John Hopfield and Dr. Geoffrey Hinton for their pioneering contributions to AI, information science is bringing about significant transformations in society and industry. Similarly, research and development that leverage information science and technology are rapidly expanding across various fields, including applied physics and semiconductor crystal research.

The application of informatics in applied physics can be broadly categorized into four main objectives: 1. Materials Informatics (MI): Efficiently predicting and discovering new materials. 2. Process Informatics (PI): Improving the manufacturing of materials and devices. 3. Measurement Informatics: Efficiently measuring and analyzing materials and devices. 4. Physics Informatics: Understanding material properties and processes. While MI has traditionally led the field, research in PI has been steadily increasing in recent years. Though MI and PI share similarities, a major difference lies in their data utilization; MI can use common databases as the parameters are standardized, whereas PI faces challenges in standardizing data due to equipment-specific parameters.

Focusing on applications in crystal growth and characterization of semiconductor materials, I will survey various research cases. Here, I aim to provide a concrete image of actual applications by categorizing data as experimental or simulated, the purpose as machine learning or optimization, and the inputs and outputs of machine learning and optimization models, along with the number of data used.

Finally, I would like to address the mindset for conducting informatics application research. The information science field has a long research history, with well-organized theories, numerous textbooks and cases, and well-prepared tools and program libraries. In recent years, sample programs can be easily obtained from the web, and powerful programming support from large language models has made adoption more accessible. However, in actual applications, it is necessary to translate the challenges faced into problems in information science. This "problem setting" is an issue in applied information science and is not yet well-systematized, with few textbooks available, and we are in a stage of accumulating individual cases. Therefore, it is important to actively introduce informatics without fear of failure and accumulate case studies. I hope this lecture serves as a catalyst for the introduction of informatics applications.

Reference

Kentaro Kutsukake, “Review of machine learning applications for crystal growth research”, Journal of Crystal Growth 630 (2024) 127598.

IT-01

Employing Plant Sourced Metals and Open Vessel Systems for Transition Metal Catalyzed Reversible Deactivation Radical Polymerization of Methacrylates

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Abstract

Transition metal mediated reversible deactivation radical polymerization (RDRP)is a robust technique to syntheize poly(meth)acrylates. It is also required to ensure the sustainability of the polymerization processes. One of the sustainable development goals (SDG) developed by United Nations Organization (UNO) is the implementation of less hazardous chemical synthesis (SDG 3). We have developed green routes employed for the RDRP of methacrylates. The major problem in this technique is the Transition metal mediated RDRP is the inevitable presence of transition metal, importantly, copper complexes. Its presence impart coloration as well as toxicity to the polymer which hinders its use in biological applications. This presentation will discuss the use of transition metals (copper and iron) extracted from green leaves as natural catalysts for RDRP. It will also discuss the efforts to develop methods to synthesize poly(methacrylates) with predetermined molecular weight and lower polydispersity index (Đ) under open vessel conditions.

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IT-02

Engineering functionalized microporous polymeric thin films for Molecular separation and energy mineral extraction

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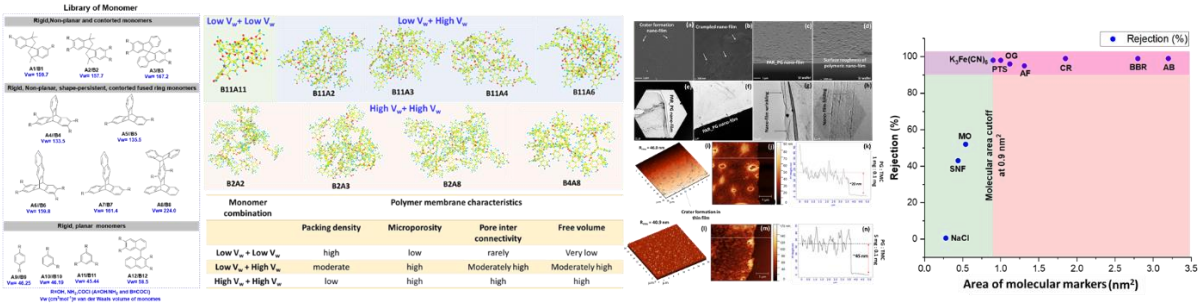
Abstract

Polymeric membranes with enhance mass-transport and solute selectivity are highly anticipated for liquid separation.[1,2] To enable membrane-based separation of a large-scale unit operation, membranes with high mass transport and solute selectivity (permeability-selectivity trade off) becomes essential to process large volume of liquids over realistic membrane area.[3]

The present work focuses on increasing mass transfer by enhancing microporosity, reducing the thickness and solute selectivity by increasing crosslinking density of the polymeric membranes. Rigid, non-planner, contorted and shape-persistent monomers that occupy high van der Waals volume (Vw) are preferred. As a function of selecting monomers with shape persistent and high van der Waals volume, we intent to restrict conformational mobility in the chain packing, allowed a structure to occupy more steric space. This enables in enhancing microporsity and interconnecting porosity. The correct choice of monomers and polymerization with a reaction kinetics assisted in producing polymeric membrane with the ultra-low thickness (~10-20 nm) and enhance microporosity. As a result, we observed enhance water mass transport as compared to the state-of-the-art the membrane without compromising solute selectivity.[4-6] Concominant separation of energy minerals[8] and controlled MWCO also achieved.[7]



Scheme 1. *Choice of monomer selection based on their van der Waals volume and Computation study of various proposed monomers combination; Thickness; MWCO*

IT-03

Type Polymer glass transition temperature (Tg): A key factor for subsurface nanoparticles

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Abstract:

Polymers attract attention from the scientific community and industry because of their unique physical and chemical properties. The research is progressing toward flexible electronics; the flexible nature of the polymers dominates futuristic electronic applications. Furthermore, for better stability, they are employed as matrix materials for the dispersion/embedding of the nanomaterials in nanocomposites. Glass transition temperature (Tg) is a special property of the polymer, at which the polymer transitions from a solid/amorphous nature to a soft, rubbery state. The present work is focused on exploring the possibility of forming sub-surface silver nanoparticles above the glass transition temperature by tuning the properties of the polymer by irradiation, doping, and blending with an interacting polymer. The optical, electrical, and morphological properties are analyzed in detail with Finite Difference Time Domain (FDTD) simulation studies. The results of the studies indicate the change in the morphology of the sub-surface particles thereby altering the properties.

IT-04

Sustainable hybrid technologies on the removal of toxic arsenic from water environment

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Abstract

Water is of vital significance to human existence. Water scarcity is really a danger to the sustainability of human society due to a growing demand. Water demand is rising owing to changes in the climate, population growth, industrialization, and destruction of the environment. To meet the demands for water, it is required to treat and reuse the waste water. Arsenic is a common ingredient that can be contained in the atmosphere, lands and minerals, aquatic life, and living species. It is an extremely toxic element that has been identified as a probable carcinogen. Arsenic pollution in marine environments is a global challenge because As-rich water can penetrate the food supply and have adverse effects on humans and other living species. Generally, arsenite is much more hazardous than arsenate. Recognizing the small levels of arsenic in drinkable water produce substantial harmful effects, methods for the elimination of arsenic are becoming highly relevant. Bureau of Indian Standards (BIS) gives the acceptable limit of arsenic in drinking water to 0.01 mg/L and in absence of other alternative sources to 0.05 mg/L. The electrochemical approach has recently drawn a great deal of interest to improved water technology, and too many studies have currently performed on this approach. The research of environmental electrochemistry has seen several advancements and achievements, as shown by the literature due to "zero pollution processing". The public desire to acquire freshwater for pollutant-free waste disposal by using biomass or by energy efficient methods, has made cleanup of industrialized wastewaters a primary focus. Electrodeionization is one the electrochemical process, which has come a long way since it, was launched commercially in 1987. Continuous Electrodeionization is a highly developed ion exchange process that combines ion exchange, electro dialysis and elusion processes for the removal of toxic metals from wastewater. Electrodeionization received more attention because there were no chemicals required for regeneration of resin, produces high pure water, economically effective processes, efficient ion removal and recovery. Electrodeionization system does have some specific benefits over all other inorganic solid, heavy metal removal techniques, like longer ion exchange resin life and membrane life compared to ion exchange processes and reverse osmosis, pollutant-free water production and complete recovery of the specified contaminant. This natural, environmentally friendly detachment approach really has a bright future, with main benefits, which encompass no chemicals needed for resin recovery, high pure water, value-effective processes, efficient ion removal and recovery.

IT-05

α-$Bi_2Mo_3O_{12}$: Functional material for electrocatalytic water splitting and supercapacitor applications.

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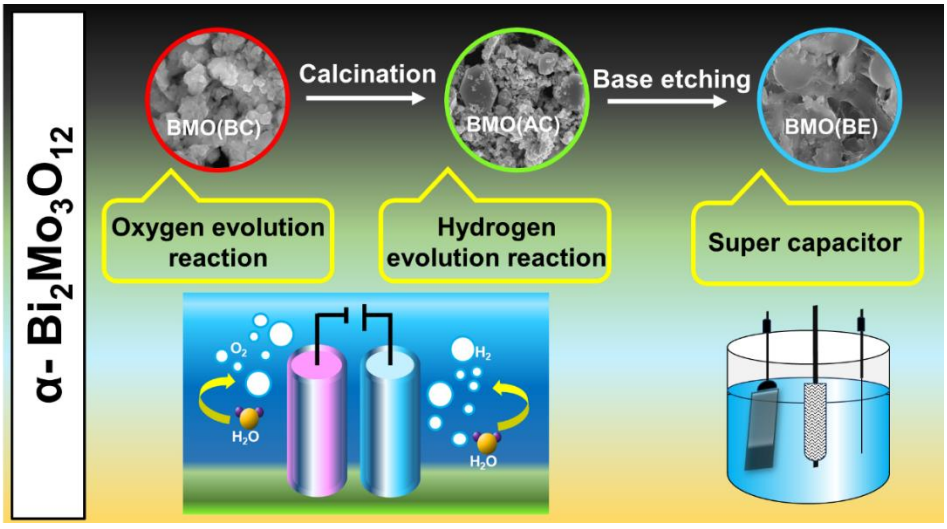
Abstract

This study explores the functionality of α-$Bi_2Mo_3O_{12}$ (BMO) as an electrocatalyst for electrocatalytic water splitting and its suitability for supercapacitor applications. BMO was synthesized by the solvothermal method and characterized in pre-calcination [BMO (BC)], post-calcination [BMO (AC)], and base-etched forms [BMO (BE)]. Structural analysis confirmed the formation of α-$Bi_2Mo_3O_{12}$ with well-defined crystallographic planes. Electrochemical analysis revealed that BMO (AC) exhibited the lowest overpotential for HER, comparable to commercial Pt-C, indicating its high electrocatalytic activity. The Tafel slope and electrochemical impedance spectroscopy results confirmed the superior kinetics and charge transfer properties of BMO(AC). Furthermore, BMO(AC) demonstrated excellent stability during prolonged chronoamperometry (CA) testing for 24h. For supercapacitor applications, the galvanostatic charge-discharge (GCD) analysis revealed that BMO(AC) is a promising candidate, achieving the highest specific capacitance value of 80 Fg^{-1} at 1.0 Ag^{-1}. Thus, the material serves as both a prominent electrocatalyst for HER and an electrode material for supercapacitor application. Overall, this study demonstrates the potential use of α-$Bi_2Mo_3O_{12}$ in various phases as a dual-functional material for efficient energy conversion and storage applications for sustainable development.

Keywords: α-$Bi_2Mo_3O_{12}$, Electrocatalysis, Supercapacitors, Overpotential, Stability



IT-06

Modeling growth of Silicene Films

Madhav Ranganathan, Nidhi Gupta and Sandipan Maitra

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Abstract

This work reports results from density functional theory(DFT) based calculations of silicene and related silicon-based structures on Ag(111) surface, followed by kinetic Monte Carlo (kMC) simulations of Silicene growth. DFT calculations are carried out using a slab model and a pseudopotential approach. KMC simulations of a lattice-based solid-on-solid model are formulated and developed in-house and simulated on parallel computers. The key surface processes are identified and their rates are estimated using energy barriers obtained from DFT calculations. Our results show that a key surface structure containing a cluster of 3 silicon atoms near each other drives the formation of 2D-hexagonal silicene sheets. The formation of silicene sheets is monitored as a function of silicon atoms at different sites on the Ag(111) surface and the cluster size variation is observed. Further efforts to model strain on the kinetics of silicene formation are part of ongoing work.

ICFMNA-25, Conference Locations

Venue: Main Auditorium

Venue: Central Seminar Hall

(ECE Annexure)

DAY 1 - 03.02.2025

ORAL SESSION

PARALLEL SESSION - I

(1.30 PM to 3.00 PM)

Venue: Main Auditorium

OP-01

Synthesis of high efficient ternary nanocomposites for photocatalysis in energy and environmental remediation

*Akshay V, Vijayalakshmi S, Sumathi Subramanian, Sasikala Ganapathy**

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Abstract

Water is considered as universal solvent due to its innate ability to dissolve more substances than any other liquid on earth. The rise in population and industrialization, there is high demand for the consumption of water for domestic and industrial needs, resulting in water scarcity and water contamination. Consequently, this tends to make the water unsafe for human consumption. In order to find solution for this environmental challenge, a facile method of photocatalytic dye degradation using visible region is employed for this work.

The main objective of this proposed work is to synthesize and characterize ternary nanocomposite by using Graphitic Carbon Nitride (g-C_3N_4), Vanadium Pentoxide (V_2O_5) and Silver nanoparticles (Ag NPs) g-C_3N_4/V_2O_5/ x% Ag (x= 3,6,9 wt.%) using simple ultrafast sonication method. The as prepared samples with varying x% of Ag is then characterized using XRD, SEM, HRTEM, Edax, FTIR and UV-Vis Spectroscopy.

The XRD pattern shows good variation in 2θ position for the prepared samples which is in accordance with the literature and JCPDS card. The SEM images shown the morphological changes of each samples. Also, HRTEM Images showcases the d-spacing and Edax shows the elemental composition of the material. The degradation efficiency of the prepared samples shows a good variation with respect to the varying weight percentage. The effective degradation of Methylene Blue (MB) dye is studied and will be discussed in full-length article. The proposed ternary nanocomposite provides an efficient tool for the removal of water pollutants from different sources during the daytime in the presence of sunlight.

OP-02

Electromagnetic Shielding Efficiency in Neodymium-Doped Doped Cu-Ni-Zn Spinel Ferrites

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Abstract

This study investigates the electromagnetic shielding efficiency (EMSE) and magnetic phase transitions of $Cu_{0.25}Ni_{0.5}Zn_{0.25}Fe_{2-x}Nd_xO_4$ ($0.000 \leq x \leq 0.100$, and $\Delta x = 0.025$) spinel nano ferrites, with a focus on the role of neodymium (Nd^{3+}) doping. These ferrites were synthesized using the sol-gel method, yielding a controlled particle size distribution and phase-pure spinel structure. Structural analysis revealed a decrease in average crystallite size from 39 nm to 15 nm with increasing Nd^{3+} concentration, attributed to lattice modifications induced by rare-earth doping. Magnetic properties, evaluated using a vibrating sample magnetometer, confirmed soft magnetic behavior. Saturation magnetization decreased from 82.69 to 66.80 emu g^{-1} with higher Nd^{3+} substitution. The reflection loss measurements in the X-band frequency range (8–12 GHz) highlighted the superior electromagnetic interference shielding and radar absorption capabilities of the $Cu_{0.25}Ni_{0.5}Zn_{0.25}Fe_{2-x}Nd_xO_4$ nano ferrites. These results demonstrate the effectiveness of Nd^{3+} doping in tailoring the structural, magnetic, and dielectric properties, making these nanoferrites promising candidates for advanced EMI shielding and radar-absorbing material applications in modern electronic and communication systems.

OP-03

One Pot Hydrothermal Synthesized BDC Templated $Cenio_3$ For High Efficiency Asymmetric Supercapacitor Electrode.

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Abstract:

Present research focused on hybrid supercapacitors based on Cerium Nickel oxide perovskite, $CeNiO_3$, and Benzene-1,4-dicarboxylic acid, MOF. Because of the fast transition of energy sources from fossil fuels to renewable ones, supercapacitors have become an alternative for storing energy, owing to their unique advantages, which include outstanding power density and long-term durability. BDC MOFs enhance the ionic transport within hybrid supercapacitors made of $CeNiO_3$, a material that has been reported to have high theoretical capacitance, excellent electrical conductivity, and improved cycle stability. The electrochemical performance of $CeNiO_3$@BDC composite was highly enhanced compared to pristine $CeNiO_3$, with a two-fold increase in capacitance, power, energy density, and cycling stability. The asymmetric supercapacitor with $CeNiO_3$@BDC as an anode and carbon black as a cathode exhibits a maximum energy density of 82.29 Wh/kg and a power density of 900 W/kg with excellent rate capability. The cycling stability tests experienced small capacitance loss in the first 2000 cycles, and stable behavior was observed afterward, which are promising for application at the large scale. Therefore, this work may be very useful in the design of electrodes in future advanced energy storage devices.

Key words: $CeNiO_3$-BDC, Perovskite, Supercapacitor, Metal organic Framework, Solvothermal synthesis, Capacitance

OP-04

Synthesis Of Binary Transition Metal Oxide V_2O_5/NiO Nanocomposite as Electrode Material For Supercapacitor Application

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Abstract

Nowadays, the lack of non-renewable energy sources and environmental pollution produced a considerable increase in the design and expansion of energy storage. Among various energy storage devices, supercapacitor plays an important role. Supercapacitors have been classified as Electric Double Layer Capacitors (EDLC), Pseudo capacitors and Hybrid according to their charge storage mechanism.

The present study is based on the synthesis of a binary transition metal nanocomposite comprising vanadium pentoxide (V_2O_5) and nickel oxide (NiO), (V_2O_5/NiO) for high-performance supercapacitor applications. These nanomaterials were synthesized by a simple and cost-effective chemical precipitation method. They exhibit high crystalline nature that can be inferred from PXRD. The functional group of the as prepared samples were examined using FTIR. The morphology of the materials was studied using SEM.

The electrochemical behaviour of the as prepared V_2O_5/NiO nanocomposite was found to be more efficient than that of V_2O_5 nanomaterial. Graphene quantum dots was also synthesized with green fluorescence and the future work aims to study the electrochemical behaviour of novel V_2O_5/NiO/GQD nanocomposite by varying the amount of graphene quantum dots (1mg, 3mg and 5mg) with V_2O_5/NiO.

OP-05

Growth of 2-Methoxy Benzoic Acid NLO Single Crystals using Vertical Bridgman Technique

Jithin Kuriakose, P. Karuppasamy *

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Abstract

NLO materials are crucial in the field development of next-generation photonic devices, frequency converters, signal processors, and optical modulator devices. There has been an increasing fascination with investigating organic compounds as NLO materials in recent years, owing to their distinctive characteristics. This research paper focuses on the exploration of 2-Methoxy Benzoic Acid as a potential sparkling substance. We explore the techniques used to create 2-Methoxy Benzoic Acid, its structural properties, and its ability to emit light when exposed to radiation. We emphasize its possible uses in detecting radiation. The Bridgman approach, a well-established method for single crystal development, was applied to manufacture high-quality crystals of 2-MBA. This process involves the controlled solidification of a molten material from an ampoule, resulting in crystals with decreased flaws and better structural integrity. The development of 2-MBA crystals was tracked under varied process parameters, including temperature gradients, pulling rates, and cooling rates. The crystal shape, size, and quality were extensively studied using optical microscopy and X-ray diffraction. The acquired results illustrate the successful growth of large, well-defined 2-MBA crystals suited for NLO applications.2-Methoxy Benzoic Acid emerges as a good candidate for organic NLO materials, demonstrating favorable structural and NLO capabilities. As the field of radiation detection continues to evolve, ongoing research and development are required to unleash the full potential of 2-Methoxy Benzoic Acid and pave the path for its practical deployment in varied applications. Also, the Bridgman approach showed to be effective in the formation of high-quality crystals of 2-MBA. The comprehensive study of these crystals emphasized their potential for NLO applications and laser technology. This research contributes to the advancement of materials for radiation detection and laser applications, creating options for further inquiry and development in these disciplines.

OP-06

A Novel Approach to Polyvinyl Alcohol Functionalized Biogenic Synthesis of Fe_3O_4 Nanoparticles For pH Responsive Delivery Of Curcumin For Cancer Therapy

*K. Vijayalakshmi[a], Dr. AL. Kavitha[a]**

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Abstract

The use of nanoparticles in cancer therapy offers many advantages due to their unique size and physical properties. In this study we have developed a formulation the surface modification of Fe_3O_4 NPs with PVA and CUR promoted the production of Fe_3O_4@PVA-CUR-NPs. The synthesized nanoparticles were well characterized by UV-Vis, FT-IR, SEM with EDX, TEM with SAED pattern, XRD, TGA and VSM to establish their physicochemical properties. Fe_3O_4@PVA-CUR-NPs., which is sensitive to cleavage at around pH 5.4, the pH of the intracellular components of endosomes/lysosomes in the cancer cell. The synthesized Fe_3O_4@PVA-CUR-NPs. exhibited enhanced drug release in lower pH conditions which mimics the cancer cell microenvironment. The cell uptake and therapeutic efficacy of Fe_3O_4-CUR nanoparticles carried out in ovarian cancer cell breast cancer cell line (MCF-7) showed improved therapeutic efficacy with Fe_3O_4@PVA-CUR-NPs.. The cell toxicity assays in MCF-7 cells indicated that pH sensitive Fe_3O_4@PVA-CUR-NPs have higher anticancer activity with IC50 at 9.2 μg/ml.

Key words: Biogenic Fe_3O_4 NPs; Curcumin; Targeted drug delivery; Cytotoxicity; Breast cancer

OP-07

$ZnAl_2O_4$ Based Nanomaterial for Sensing Application

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[2] Department of ECE, Swarnandhra College of Engineering and Technology, Narsapur, A. P., India

Abstract

This study presents the X-ray response and optical properties of Zn (1-x) Al_2O_4Tix composite nanoparticles made via a straightforward, economical sol-gel process, subsequently sintered at 700°C. X-ray diffraction verifies the polycrystalline structure comprising hexagonal and cubic phases, exhibiting favoured grain orientations along the (311) plane for $ZnAl_2O_4$ and the (101) plane for ZnO. Raman spectra exhibit pronounced vibrational peaks of TiO_2 at 143 cm^{-1} and 391 cm^{-1}. Analysis of surface morphology reveals spherical granules with an average diameter of 87.16 nm. Elemental analysis verified the existence of Zn, O, Al, and Ti. The sample's absorbance at 333 nm and an optical band gap of 3.72 eV indicate its appropriateness for economical sensor applications.

OP-08

Radiation Sensing Application for Groundwater Analysis: A Data-Driven Approach

Krishna Koushik[1], S Mullai Venthan[2], Pooja Gowda[1]*

[1]Department of Computer Science and Engineering, Amrita School of Computing, Amrita Vishwa Vidyapeetham, Bengaluru, India.

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Abstract

Employing both Exploratory Data Analysis (EDA) and Data Visualization (DV) methods, these findings offer a clear view of inherent multivariate relationships within the dataset validating ML-based predictions. The general measurable aspects play a significant role in the accurate measurement of radioactive compounds in underground water and stresses the negative effects of radioactive substances on health and the environment. As can be evidenced from this combined approach, improvements in the state of the art in ML approaches when augmented by the expertise of domain specialists when dealing with large–scale data result in more accurate and flexible models that we are able to generalize. The proliferation of big data in different fields has therefore impeded the applicability of ML methods for extracting meaningful information. However, applying this idea of dimensionality reduction for maximum model performance is not as straightforward due to some peculiar problems, including noise, irrelevant features, and overfitting problems. This research focuses on applying sound data pre-processing, feature extraction, and relative comparison of multi-faceted ML methods for dealing with the Noise and irrelevant features in data, Overfitting in predictive modeling, High dimensional data. Using various performance metrics that include accuracy, precision, and recall values, the work carried out on underground water data sets with parameters including uranium, thorium, and radium concentrations emphasizes the fact that cleaning data, engineering features, and clustering are critical in enhancing the predictive capability and generalization of any model. In addition, it puts forward possible future research agendas regarding distributed optimization methods to increase the ML model performance in high-risk applications.

OP-09

Investigation Of Structural, Geometrical and Electronic Properties of Xbi_2o_5 (X= Ti, Ge, Mg) By First Principles Calculations

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Abstract

The structural, geometrical and electronic properties of XBi_2O_5 (X = Ti, Ge, Mg) are analyzed using first-principles calculations. BURAI 1.3, a graphical user interface designed for the Quantum ESPRESSO (QE) software package, was used to analyze the Kohn–Sham equations employed in these calculations, which were performed using the density functional theory (DFT) approach. Ultrasoft Pseudopotentials (USPPs) were used to implement the Generalised Gradient Approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) functional in order to address the exchange–correlation term of the Schrödinger equation. The crystal structure was optimized, and the ground-state energy was calculated using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) optimization technique. The simulated structures consist of a primitive 1×1×1 supercell in the orthorhombic phase. The cut-off energy, optimized convergence standards and k-grid points were applied for self-consistent field (SCF) calculations. The total energy and fermi energy were determined after a SCF calculation. The calculated equilibrium lattice parameters are used to plot the band structure and Density of States (DOS) diagrams.

OP-10

Anticancer activity of Phyto-fabricated Copper nanoparticle using *Cestrum aurantiacum* aqueous extract against colon cancer

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ksareen114@gmail.com

Abstract:

The advancements in science and technology have led to the exploration of nanoparticle-based drug formulation. This has the potency to better treat the patients with solid tumors such as colon cancer. According to the current statistics incidence rate of colon cancer in India is relatively low at 7.2 per 100,000 population for men and 5.1 per 100,000 for women. It is ranked as the 7th most common cancer in India with a 5-year survival rate below 40%. Copper is FDA approved metal for use in humans with many advantageous pharmacological features. Phyto-fabrication, the use of plant extract, in the synthesis of nanoparticle has advantages such as being less toxic, environmental-friendly, and incorporation of bioactive plant ingredients in the synthesized nanoparticles. The aqueous extract of *Cestrum aurantiacum* was used in the green synthesis of copper nanoparticle. The characterization studies such as UV-Vis Spectrophotometry, FTIR, SEM and XRD confirmed the presence of crystalline copper nanoparticle ranging from 30-50nm in size. The DPPH assay showed that the maximum radical scavenging activity was obtained at a concentration of 1000µg/ml. The minimum inhibitory concentration (IC50) against HT 29, a colon cancer cell line was obtained at 121.06µg/ml. The Phyto-fabricated copper nanoparticles from the flowers of the plant *Cestrum aurantiacum* exhibited promising results in the inhibition of cancer cell lines like HT-29 using MTT assay. The anticancer activity of the copper nanoparticles was very much similar to the commercially available anticancer drugs like vincristine, doxorubicin, carboplatin, etc. Hence, the Phyto-fabricated copper nanoparticles can be clinically developed and used as anticancer agents.]

PARALLEL SESSION - I

(1.30 PM to 3.00 PM)

Venue: Central Seminar Hall

(ECE Annexure)

OP-11

Biodegradable Polymers for Food Packaging: PLA Film Technology as a Green Solution for Banana Packaging

Shreya Vivek, Yamini Tholeti, Nithya Amineni, Kavya Javvaji, Shwethaa V, Vinoth Kumar V

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Abstract

Food packaging plays a crucial role in maintaining quality, extending shelf life, and reducing waste. With growing demand for sustainable solutions, biomaterials like polylactic acid (PLA) offer eco-friendly alternatives to conventional plastics like polyethylene (PE). This study explores PLA bioactive films as effective, sustainable food packaging using Poovan bananas as test subjects due to their uniform ripening and compact size. The study monitored ripening progression through biochemical markers (e.g., starch breakdown, sugar content, antioxidant activity, titrable acidity, TSS), analytical methods (GC-MS), and visual assessments (peel discoloration, shrinkage, weight loss). Six film types were tested: plain PLA, PLA infused with chitinase (antimicrobial), PLA with rhamnolipids and essential oils (antimicrobial/antioxidant), and PLA combining all three additives. Comparisons were made with PE film and an unwrapped control group to evaluate natural ripening. PLA with rhamnolipids and essential oils showed predominant values as expected, with a decrease in overall weight but a starch content thereby indicating a steady and better alternative as a food packaging material with high-end properties as compared to the hazardous polyethylene (PE). The study highlights the potential of PLA bioactive films in reducing food waste and enhancing storage efficiency.

OP-12

Synthesis, spectral characterization, DFT-Computational analyses on Novel 2,4-dichlorobenzoic acid P-dimethylaminobenzaldehyde (DBADAB) single crystal study

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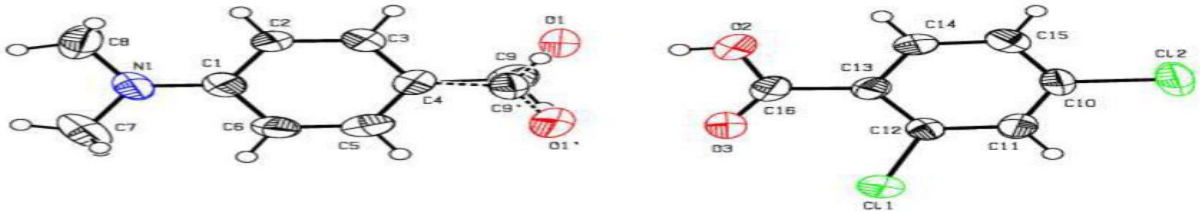

Molecular structure of the compound with 50% probability thermal displacement ellipsoids

Abstract

A novel third-nonlinear optical (NLO) crystal, p- (dimethyl amino) benzaldehyde 2,4-dichlorobenzoicacid (abbreviated as **DBADAB**) was successfully synthesized and grown good quality crystal by slow evaporation solution growth technique by methanol as a solvent at room temperature. The formation of the grown crystal was carried out by single-crystal X-ray diffraction analysis. The powder X-ray diffraction study was completed, and the peaks were indexed. The recorded UV spectrum gives two absorption peaks, one at 331nm. The band gap energy calculated, and it is found to be Eg = 3.7eV which shows suitable applications of the optoelectronic device. In the photoluminescence study, the broadening violet emission band at 414 nm is assigned to π – π* transitions of the C=O groups present in the compound. The functional groups of the grown crystal have been determined by Fourier Transform Infra-Red (FTIR) spectroscopy technique. In thermogravimetric (TGA) and differential thermal analysis (DTA) analysis, the title material was determined as thermally as stable up to 234 °C. The Vickers Microhardness test ascertained the mechanical properties of the grown crystal material, and it belongs to a soft material category. The dielectric measurements of the developed crystal material were also as- certained at various frequencies. The dielectric constant, dielectric loss, and A.C. the conductivity of title material was studied with different frequencies and temperatures. The laser damage threshold (LDT) of the grown crystal was then calculated by using Nd: YAG laser. The grown crystal has given the measured (LDT) value of 8.97 GW/cm 2 . The third-order nonlinear optical (NLO) properties characteristics, such as absorption coefficient (β~0.09 $\times 10^{-4}$ cm/W), the refractive index (n_2 ~ 5.5210 $\times 10^{-8}$ cm 2 /W), and their susceptibility range values of (χ(3) ~3.46 $\times 10^{-6}$ esu) of the grown crystal was estimated by Z-scan tech- nique, suggests that the grown crystal material **DBADAB** was served as a promising source for nonlinear optical devices.

Keywords: Novel (**DBADAB**) crystal, Spectral characterization, DFT-Computational analyses, biological studies.

OP-13

Performance And Mechanism of Lead Removal Using Sludge Based Biochar Loaded With Zerovalent Iron

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Abstract

Heavy metal contamination, particularly lead (Pb), poses a severe threat to environmental and human health due to its toxicity and persistence in water systems. Sludge management is a pressing global issue, driving increased focus on environmentally sustainable and eco-friendly treatment solutions. This abstract explores the innovative utilization of sewage sludge biochar (SSB) loaded with zerovalent iron (ZVI) for the adsorption of Pb from aqueous solutions. The approach leverages the dual functionality of biochar as a sorbent and ZVI as a reductant to achieve efficient lead removal, demonstrating a sustainable application for waste-derived materials in water treatment. The sewage sludge was pyrolyzed at varying temperatures to produce biochar with optimized surface characteristics. The biochar was subsequently impregnated with ZVI nanoparticles via a chemical reduction method, enhancing its adsorption efficiency and reactivity. Zerovalent iron (ZVI) exhibits a high surface area, especially in its nanoscale form, which enhances its adsorption capacity. Its reactive surface contains active sites and functional groups that facilitate the binding of contaminants like heavy metals. Additionally, its reductive potential enables simultaneous adsorption and reduction, improving the efficiency of pollutant removal. Results revealed that the ZVI-loaded biochar exhibited significantly higher Pb adsorption capacity compared to unmodified biochar, with removal efficiencies exceeding 95% under optimal conditions. The composite material's high surface area, functional groups, and synergistic effects between ZVI and biochar were identified as key contributors to its performance. This study highlights the feasibility of utilizing waste-derived materials for environmental remediation and provides valuable insights into the mechanisms of Pb removal, paving the way for more sustainable and cost-effective solutions in wastewater treatment.

OP-14

Facile synthesis of Fe-UiO-66 MOF for efficient photodegradation of antibiotics under visible light.

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Abstract

Water pollution has become a global issue, driven by rapid industrialization, urbanization, and population growth, leading to severe environmental degradation. Pharmaceutical contaminants, particularly antibiotics, have emerged as a critical environmental threat due to their extensive usage and improper disposal. To address this challenge, the Fe-UiO-66 Metal organic framework was successfully synthesized via solvothermal method. Further, the prepared materials were characterized by subjecting them to X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Fourier-transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), UV-vis spectroscopy, scavenger tests, and stability evaluations. These analyses revealed that Fe-UiO-66 consists of agglomerated irregular spherical particles with robust structural stability and a smaller band gap. The Fe^{3+} ion doping on the surface of UiO-66 significantly enhanced the physiochemical and photocatalytic properties by improving electron transfer efficiency and minimizing electron-hole pair recombination. The prepared material exhibited superior photocatalytic efficiency in the degradation of tetracycline hydrochloride under visible light irradiation. The remarkable stability, retaining its performance upto five cycles. These findings highlight the potential of Fe-UiO-66 metal organic framework sustainable and highly efficient photocatalysts for wastewater treatment.

OP-15

Waste Water Segregation using Nanomaterials and Machine Learning Classification Models

Manjunath[1], S Mullai Venthan[2], Pooja Gowda[1]*

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Abstract

Water treatment and wastewater isolation are major issues that world needs to think about to help reduce scarcity of water and manage the environment. Some of the studies preceding the present work have investigated the application of nanomaterials in the context of wastewater purification with an emphasis placed on the improvement of contaminant adsorption/ separation. However, the current studies have some drawbacks such as limited scalability; low generalization to real-world conditions and slow performance concerning a wide variety of wastewater types. ML techniques have been used for enhanced predictive accuracy and effective treatment of many ailments, but, to the best of our knowledge, the integration of nanomaterials with ML models has not been properly explored for effective wastewater treatment. This research fills this void by using machine learning models including Random Forest, Support Vector Machines and Neural Networks in prediction models of nanomaterials in the experimental studies to determine the best practices for wastewater segregation beside preprocessing techniques with feature engineering, sampling techniques. The dataset contains 107 records and has 23 attributes where it contains significant information regarding different types of nanomaterials affects the properties like the time dependent absorbance. These include: TiO_2, H_2O_2, $K_2S_2O_8$, $NaIO_4$, and silver with their doses, reaction times intervals, and absorbance taken under various experiments. Through the use of this structured data set the study improves the understanding of nanomaterial interactions and transformations within chemical and environmental processes. The presented outcomes show enhanced efficiency, lower cost, and adaptability to larger volumes of wastewater as compared to traditional water treatment technologies and their potential as a sustainable solution for wastewater treatment.

OP-16

Cobalt-based ternary Semiconductors for Energy Recycling Applications

*Klinton Brito K[1], M Srinivasan**

Department of Physics, SSN Research Centre, Sri Sivasubramaniya Nadar College of Engineering, Kalavakkam

Abstract

XCoP (X=Ti, Zr, Hf) half Heusler alloys are investigated through density functional theory in stable non-magnetic phase. The exchange-correlation functional Generalized Gradient Approximation (GGA) is used to study these alloys. The equilibrium lattice constants and corresponding ground state energies of the studied alloys are calculated in stable γ-phase. All these three reported alloys exhibit semiconducting behavior with corresponding bandgap values of 1.40, 1.29, and 1.38 eV for TiCoP, ZrCoP, and HfCoP, respectively. The studied alloys are mechanically stable and ductile in nature. The obtained thermoelectric figure of merit for p-type TiCoP, ZrCoP and HfCoP are 0.5, 0.6, and 0.7 at 1200 K. Similarly, the figure of merit obtained for n-type TiCoP, ZrCoP, HfCoP are 0.54, 0.37, and 0.31, respectively, at the same temperature. The investigated favorable transport properties of these alloys show that they are the potential candidates for waste heat energy harvesting application.

OP-17

Eco-Friendly Nanocomposites from Biowaste: Metal-Doped Hydroxyapatite and Polymer-Based Coatings for Biomedical Applications

M. Jeevadharani[a] E. Gunashree[b] M. Surendiran[a]*

[a]Department of Chemistry, School of Arts and Science, Vinayaka Mission's Chennai Campus, Vinayaka Mission's Research Foundation, Paiyanoor, Chennai- 603 104.

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Abstract

In recent years, there has been a growing focus on developing nanomaterials from biodegradable waste to support eco-friendly advancements. Crab shells, a significant source of calcium carbonate ($CaCO_3$), have been effectively utilized in the synthesis of hydroxyapatite (HAP), a biomaterial valued for its biocompatibility, biodegradability, and non-toxic characteristics. The unique crystal structure of HAP, coupled with its ease of synthesis, makes it highly suitable for biomedical applications. Incorporating metal dopants, such as ytterbium (Yb) and niobium (Nb), into HAP, along with biopolymers chitosan derived from prawn shells, has demonstrated considerable potential for implant technologies. These composites, when deposited on surface-treated Ti6Al4V titanium alloys using the electrophoretic deposition technique, exhibit enhanced corrosion resistance and mechanical stability, critical for bone implants. Titanium alloys, particularly Ti6Al4V, are preferred in this domain due to their excellent biocompatibility and minimal modification requirements. Advanced characterization techniques, including FTIR, XRD, SEM,XPS, thermal studies and contact angle measurements were employed to evaluate the coatings functional groups, crystalline phases, surface morphology, wettability, and corrosion resistance. The coatings further demonstrated antimicrobial efficacy against gram-positive and gram-negative bacteria, highlighting their potential to reduce infection risks in bone applications. To enhance the structural and functional properties of the composites, polymers were integrated as fillers, creating robust materials with mechanical and biological characteristics closely resembling natural bone. This composite structure effectively mimics human bone tissue, making it a promising candidate for advanced orthopedic and dental implants.

OP-18

Conformational Energy Profiling of Clopidogrel Bisulfate in the Gas Phase Using DFT Calculations

Roselin Pavithra A [1], Ramesh P [2], S.I. Davis Presley [3*], M. Srinivasan [4]*

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Abstract:

This study presents a comprehensive theoretical investigation of Methyl (+)-(S)-O-(2-chlorophenyl)-6,7-dihydrothieno[3,2-c]pyridine-5(4H)-acetate hydrogen sulfate, commonly known as Clopidogrel bisulfate ($CPG.H_2SO_4$), an antiplatelet agent. Unlike previous Density Functional Theory (DFT) studies that examined clopidogrel base and sulfuric acid individually, our research focuses on the combined bisulfate molecule. Employing the B3LYP method with the 6-311+G (d, p) basis set, we analysed the molecule's molecular structure, vibrational properties, thermodynamic characteristics, and Frontier Molecular Orbitals (FMO). The HOMO-LUMO analysis revealed critical information on charge transfer potential, band gap, and pharmacological relevance. The C3 conformer emerged as the most stable structure with the lowest energy, exhibiting notable electron-withdrawing behaviour. Electrostatic potential (ESP) analysis provided valuable insights into electron distribution and potential reactive sites. These findings contribute to a deeper understanding of $CPG.H_2SO_4$'s drug-receptor interactions and its pharmacological profile.

Keywords: Clopidogrel bisulfate, Density Functional Theory (DFT), B3LYP, vibrational analysis, electrostatic potential (ESP).

OP-19

Synthesis of spongy spherical NiB/B-rGO nanocomposite using hydrothermal method for high-performance supercapacitors

E Murugan & Vinitha Annachi*

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Abstract

Extensive global research into energy conversion and energy-storage technologies, more especially in the area of nonconventional energy sources, has been made possible by the quick depletion of non-renewable energy supplies. The development of different storage devices, particularly energy-storage devices include supercapacitors (also known as electrochemical capacitors, EC), batteries, etc., has been the subject of much study. Although electrochemistry plays a crucial role in batteries as well in supercapacitors, their energy and power densities were differed. Crucially speaking, transition metal borides show higher conductivity, thermoelectricity, magneticity, and field-emissivity. The benefits of using carbon materials are good electrical conductivity, easy manufacture, high chemical stability, higher specific area, good electrical conductivity, easily abundance and wide working temperature range. In this work, the synthesis of nickelboride/boron doped rGO (NiB/B-rGO) was carried out by hydrothermal method and the products were characterised with XRD, Raman spectroscopy, FT-IR, SEM and XPS. The electrochemical performance of the NiB/B-rGO was analysed using cyclic voltammetry (CV), galvanostatic charge-discharge (GCD) and electrochemical impedance spectroscopy (EIS). The specific capacitance of synthesised NiB/B-rGO nanocomposite is 1012.72Fg^{-1} at 1Ag^{-1} with energy density 42.16 Wh kg^{-1} and power density 272.48 W kg^{-1}. The NiB/B-rGO nanocomposite could be a convenient choice as electrode materials for the fabrication of commercial supercapacitors in the future.

OP-20

Facile Synthesis of $NiCo_2S_4$ for Visible Light Driven Organic Pollutant Degradation.

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Abstract

Recent modernization has spurred economic growth but has also escalated water pollution. In addressing this challenge, photocatalysis utilizing various photocatalysts have shown huge promise for effective and energy-efficient organic wastewater degradation. In this study, Nickel Cobalt Sulphide ($NiCo_2S_4$) was synthesized by facile solvent-free calcination process. The structural characteristics and their variations were analysed using X-ray Diffraction (XRD) and Fourier Transform InfraRed (FT-IR) analyses. The chemical coordination and optical properties were investigated by X-ray Photoluminescence Spectroscopy (XPS) and Ultraviolet-Visible (UV-Vis) spectroscopy, respectively. $NiCo_2S_4$ exhibited a bulk, plate-like morphology, as observed in Scanning Electron Microscopy (SEM) and Energy Dispersive X-ray Analysis (EDAX) analysis confirms the presence of all elements. The photocatalytic degradation efficiency of the as-prepared material was evaluated using Congo Red (CR) dye under visible light irradiation. It also showed excellent stability over five cycles, making it a viable and cost-effective candidate. Thus, this material holds significant interest for the sustainable degradation of organic pollutants, offering a potential solution in future wastewater degradation.

OP-21

Microwave assisted synthesis of PTHOB decorated with gC_3N_4 and rGO for Supercapacitor Application.

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Abstract

The storage of energy in this technological world we live in, is at high stake hence; to store it efficiently, researchers have been exploring new materials and methods recently. Supercapacitors being promising candidates to store electrical energy as solid-state device with high power density, quick charge–discharge time, low input resistance, extended cyclic stability may overcome many of the drawbacks in batteries. Thus, synthesis of new electrode materials with efficiency is considered to be paramount significance and order of the research retrospective literature survey reveals that in supercapacitors, organic conjugated polymers had displayed remarkable multifunctional characteristics. Therefore, in line with the literature this work aims for a microwave assisted synthesis of Polythiophene derived Polythiophene-co-hexyloxybenzene (PTHOB) decorated with gC_3N_4 and rGO. The as synthesised polymeric materials were characterised using FT-IR, RAMAN, and NMR spectroscopic techniques. Electrochemical studies using cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectra (EIS) were conducted to investigate the electrochemical characteristics and capacitance of the same. Wherein, the specific capacitance of 443 F/g at 1 A/g with energy density 55.375 Wh/Kg and Power density 450 W/Kg is achieved for the control material. Comparative study is done to analyse the electrochemical activity of the other composite materials with the control which yielded an improved capacitance proving to serve as promising materials for energy storage. Thus, the results of the application could be highly performable, which would become the future of energy storage devices.

OP-22

Solvothermal Synthesis of CoS/rGO nanocomposite for supercapacitor application

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Abstract

The ever-growing energy demands and deteriorating environmental situations call for green and more sustainable energy storage systems. Researchers have been focusing on the alternative energy storage device to overcome the energy demand. Recently, supercapacitors(SCs) are one of the promising energy storage devices. However, SCs utilize fast surface processes to store charges and have low energy density, so in order to meet the demands of application scenarios that have elevated power and energy density needs, storage devices for energy with superior performance must be developed. High-performance electrodes materials must be created in order to improve the electrochemical functionality of SCs, hence sulphur-based nanocomposite materials have a significant impact on the mechanism for storing energy and performance metrics of SCs. This abstract shows the synthesis, characterisation and electrochemical studies of CoS/rGO nanocomposite for energy storage supercapacitor application. The nanocomposite was characterised using different techniques like XRD, FTIR, Raman and SEM. The electrochemical studies were done using CV, GCD and EIS techniques in 3M KOH as an electrolyte aqueous solution. The specific capacitance of the CoS/rGO nanocomposite is 1421 Fg^{-1} at $1Ag^{-1}$ current density. The energy density is 49.02 Wh kg^{-1} and power density of 249.96 W kg^{-1}. The cyclic stability of the CoS/rGO nanocomposite was 78.3% after 1000 cycles. The CoS/rGO prepared nanocomposite shows very high specific capacitance so that it could be a promising electrode material for the fabrication of energy storage devices in real life energy storage applications.

OP-23

Hybrid Smart Grid Storage System with AI-Optimized Thermal and Battery Management

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Abstract:

Optimal energy management in complex power systems of the present world requires the incorporation of advanced energy storage systems and intelligent optimization algorithms. The hybrid smart grid storage system integrates the latest technologies including vanadium redox flow batteries for daily cycling, hydrogen-based power-to-gas systems for long-term storage, and molten salt batteries for peak energy storage. These storage systems solve the problems associated with rising renewable energy integration, grid balance, and reliability under varying conditions. AI is central to enhancing the system performance by controlling the real-time energy dispatch, scheduling of maintenance, and dynamic thermal management. They improve productivity, increase the durability of operational equipment, and minimize disruption of service delivery. In storage itself, the integration of storage and generation resources can effectively control the load and renewable generation. The analysis of different machine learning models provides insights into thermal and battery characteristics. Decision Tree is identified as the best model for thermal systems, giving the lowest MSE, RMSE, and high R^2. Likewise, linear regression models are outstanding in battery performance, providing an almost perfect forecast with an R^2 of 1.0 and negligible error. Random Forest & the Decision Tree attained the highest feasible scores of 1.0 for overall performance metrics measured across models for overall model reliability for real-world energy management systems. The proposed hybrid system efficiently integrates various types of energy and utilizes the opportunities of innovative storage and AI optimization. This approach does not only solve present day to day operational issues but also fosters the future of grid reliability and stability, which is a key element of a more sustainable energy system. Such outcomes raise the possibility of combining intelligent storage systems with renewable energy to transform the contemporary power systems.

OP-24

Prediction of Logarithmic breakdown field in Dielectrics using Machine learning Techniques

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Abstract:

The ability to predict the logarithmic breakdown field in dielectric material is a major task in the design of electronic products. Breakdown fields define a material's endurance towards electric stress. Breakdown field can directly measure the reliability and functionality of dielectric materials depending on environmental and operating conditions. Conventional approaches for estimation of breakdown fields primarily depend on empirical equations and theoretical models. These methodologies suffer from certain assumptions and fail to account for the non-linearities that can exist in material properties. The breakdown filed can be analyzed by emphasizing the influence of material properties. The dielectric breakdown field being highly nonlinear and dependent on multiple parameters such as structure, density and category of the material. Machine learning (ML) algorithms are used to analyze the logarithmic breakdown field of dielectric materials as they high capability of analyzing high-dimensional data and identifying nonlinearity. The variations in material composition, structure and processing methods that influence breakdown field are analyzed using SMOTE and quotient of determination is observed to be 94%.

Keywords: Logarithmic breakdown, Dielectric materials, Machine Learning, SMOTE

OP-25

Reinforcement Learning-Based Framework for Nuisance Alarm Reduction in ϕ-OTDR-Based Perimeter Intrusion Detection Systems

- Abisri S

Abstract

Perimeter intrusion detection systems (PIDS), particularly those utilizing ϕ-OTDR technology, rely on critical performance metrics such as probability of detection (POD), nuisance alarm rate (NAR), and false alarm rate (FAR). While substantial advancements have been made in detection accuracy, mitigating the nuisance alarm rate (NAR) without degrading detection sensitivity remains a key challenge, especially in noisy, dynamic environments. This paper introduces a novel reinforcement learning (RL)-based framework tailored for continuous state spaces to address this issue. By leveraging RL, the system learns an optimal policy to minimize NAR while maintaining high sensitivity. The proposed approach combines advanced data denoising techniques with an RL-based decision-making model, enabling improved differentiation between genuine events and irrelevant noise. Experimental results demonstrate a significant reduction in NAR and enhanced overall system reliability for fibre-optic-based intrusion detection systems.

DAY 1 - 03.02.2025

ORAL SESSION-II

(4.50 PM to 5.30 PM)

Venue: Main Auditorium

OP-26

$ZnAl_2O_4$ Nanoparticles via Sol-Gel Synthesis: A Gateway to Wireless Applications

Narayana LVS, Ribhu Abhusan Panda, Srilali Siragam[*]

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Department of ECE, Swarnandhra College of Engineering & Technology, Narasapur, A.P [3]

Abstract:

Researchers are now investigating suitable dielectric materials to meet the demand for miniaturized and lightweight wireless microstrip patch antennas. Nanoparticles of zinc aluminate ($ZnAl_2O_4$) have a low loss and a high dielectric permittivity, making them ideal for use in microwave applications. This paper details the chemical composition, morphology, structural and dielectric properties of $ZnAl_2O_4$ nanoparticles synthesized using a sol-gel technique. Crystallinity of the prepared nanoparticles was 19.5 nm for ZnO wurtzite. Further, we measure the dielectric permittivity at 30, 40 and 50 °C, with results of 8.82, 8.80 and 8.78 respectively. With recorded values of dielectric loss were 0.06, 0.04 and 0.05, the prepared nanoparticle was found to decrease with increasing frequency.

OP-27

A Computational Investigation Of Structural, Mechanical, Electronic, Thermoelectric And Optical Properties Of TiPdZ (Z=Al,Ga And In) Half-Heusler Alloys

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Abstract:

Half-Heusler (HH) alloys are at the forefront of thermoelectric research, offering a unique platform to convert waste heat into usable electricity due to their inherent semiconducting properties and thermal stability. In this study, we present a comprehensive theoretical investigation into the thermoelectric performance of Half-Heusler compounds using first-principles density functional theory (DFT) coupled with Boltzmann transport equations. By systematically exploring the effects of elemental substitution and doping at specific lattice sites, we analyze their influence on electronic band structures, carrier effective masses, and thermal conductivity.

Our findings reveal that tailored chemical modifications can significantly enhance the power factor by optimizing the Seebeck coefficient and electrical conductivity. Moreover, phonon transport calculations highlight the role of mass disorder and anharmonic interactions in reducing lattice thermal conductivity, thereby improving the figure of merit (zT). These results provide critical insights into the design principles for high-performance Half-Heusler thermoelectric materials, paving the way for their application in energy harvesting systems, including industrial waste heat recovery and sustainable power generation. This work underscores the transformative potential of theoretical approaches in accelerating the development of next-generation thermoelectric materials, aligning with global energy efficiency goals.

OP-28

Affordable Optimizing Anode Materials infused Recycled Silicon for Highly Stable Lithium-Ion Batteries

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Abstract:

Pencil lead, composed of a mixture of graphite (Gr), silica (SiO_2), and clay, is widely utilized for writing, sketching, and technical drawing, and it can exhibit characteristics similar to other graphite-based materials. This study introduces a straightforward method to prepare a Gr/SiO_2 composite anode material using pencil lead. Hydrochloric acid (HCl) is employed to eliminate the wood and impurities from the lead. Subsequently, the purified pencil graphite is finely ground using a mortar and pestle. The resulting graphite is mixed with a cleaned and processed silicon (Si) kerf slurry waste, produced during the cutting and wafering of multi-crystalline silicon ingots, to create an anode material suitable for lithium-ion batteries. The kerf silicon composites, at the concentrations of 4%, 5%, and 12B pencil graphite treated 5% kerf silicon @ 850°C electrode produced a specific capacity to 258 mAh g^{-1} after 1000 cycles, with galvanostatic charging and discharging conducted at a current density of 1000 mA g^{-1}. X-ray diffraction (XRD), Raman spectroscopy, and field-emission scanning electron microscopy (FESEM) were used to conduct a comprehensive analysis of the pencil lead powder. These electrodes appear to be potentially effective and cheap energy storage devices considering the consistent stability in potential and elevated discharge capacities noted during galvanostatic charge-discharge experiments.

Keywords: pencil lead Recycle silicon, anode, lithium-ion battery.

OP-29

Chemical Depolymerization of Waste Polyethylene Terephthalate into Value-added Products

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Abstract:

Plastic waste poses significant environmental challenges due to its non-biodegradable nature and the release of harmful pollutants when incinerated. Thermocatalytic depolymerization (TCDP) has emerged as a promising approach to convert post-consumer plastic waste, such as polyethylene terephthalate (PET) and polycarbonate (PC), into valuable products. Organocatalysts are preferred over metal-based catalysts for their environmental friendliness. In this study, two organocatalysts such as L-proline: trifluoroacetic acid (TFA) and morpholine: TFA were synthesized and thoroughly characterized.

The TCDP process utilized these synthesized organocatalysts, commercial L-proline, and Y_2O_3 as effective catalysts for the glycolysis (using ethylene glycol (EG) as the reactant) and aminolysis (using ethanolamine (EA), allylamine (AA), and m-xylene diamine (XD) as reactants) of waste PET. The depolymerization of PET yielded bis(2-hydroxyethyl) terephthalate (BHET) (66.21–80%), PET oligomers (30%), N^1, N^4-bis(2-hydroxyethyl) terephthalamide (BHETA) (87%), N^1, N^4-diallyl terephthalamide (DATA) (93.7%), and N, N'-bis(3-(aminomethyl) benzyl) terephthalamide (BAMBTA) (91.69%). Similarly, glycolysis of waste PC effectively recovered bisphenol-A (BPA) with a yield of 83%.

The recovered BPA and BHET were subsequently used as monomers and co-monomers for the synthesis of high-performance polycarbonate (PC) and co-polycarbonate (Co-PC) via a polycondensation method. This process improved the thermal properties of the polymers, notably enhancing their degradation temperature (T_d).

OP-30

X-ray Photoelectron spectroscopy of Sb_2O_3 and Fe_2O_3

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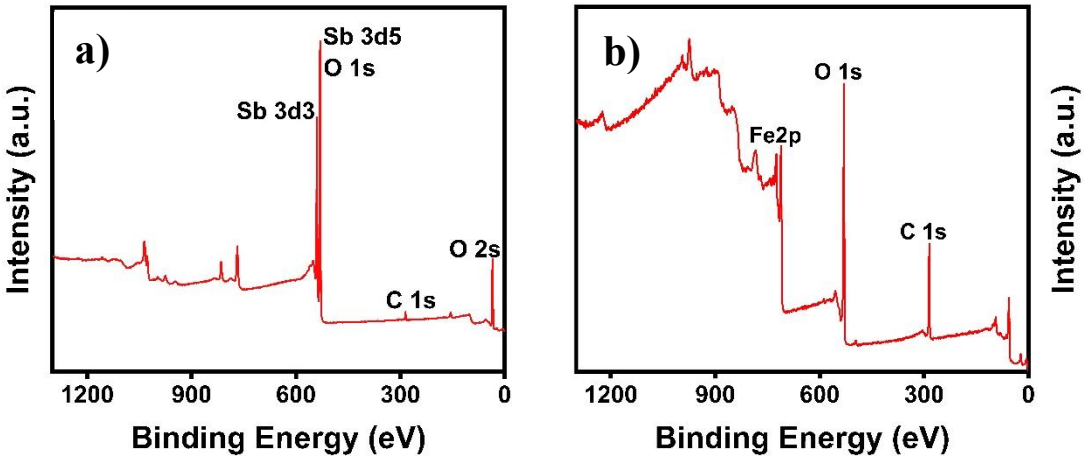
Abstract

X-ray photoelectron spectroscopy (XPS) is a surface analytical technique used to analyse the surface chemistry and composition of materials. In this research work commercial single phase Sb_2O_3 and Fe_2O_3 materials was characterized using XPS technique to understand chemical bonding, binding energies, composition and impurities. Priorly both the polycrystalline samples were characterised for its structure, morphology, and X-ray shielding nature. These experimental findings will be discussed in det



Survey spectrum of (a) Sb_2O_3 and (b) Fe_2O_3

OP-31

Synthesis and Stabilization of Fe_3O_4 Nanoparticles and Evaluate their compatibility and Biosensor Applications

Sibisudhan S

Abstract:

The study focuses on the synthesis and stabilization of magnetite (Fe_3O_4) nanoparticles for their biocompatibility and biosensor applications. Magnetite nanoparticles, known for their superparamagnetic properties and biomedical potential, were synthesized using the co-precipitation method. The nanoparticles were stabilized with hydroxylpropyl methylcellulose (HPMC), a biocompatible polymer, to prevent coalescence and enhance their functional properties. The synthesized nanoparticles were optimized and characterized using UV-Vis, FTIR, TEM, SEM, and TGA analyses, revealing effective stabilization and dispersion dependent on HPMC concentration.

Composite films of HPMC and magnetite nanoparticles were prepared, showing variable color and sedimentation based on polymer-to-nanoparticle ratios. UV-Vis spectroscopy confirmed the successful formation of magnetite nanoparticles and indicated their integration into HPMC biocomposites. The ongoing work is the development of a biosensor film aimed at detecting Fe^{2+} content in blood, with potential applications in real-time wearable devices for biomedical diagnostics.

OP-32

Synthesis of $Cd(OH)_2$-CdO Nanoparticles Using Veldt Grape Leaf Extract: Enhanced Dye Degradation and Microbial Resistance

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Abstract

This research work implies the development of a reliable, inexpensive, better and eco-friendly way to fabricated $(OH)_2$ and CdO nanoparticles green synthesis approach using three different source materials. The *veldt grape leaf* act as a chelating agent. The physical properties of prepared samples were analyzed by various characterization techniques such as X-Ray Diffractometer, Fourier Transform Infra-Red, Scanning Electron Microscopy, X-Ray Energy Dispersive Spectrometer, High-Resolution Transmission Electron Microscopy andUV-Visible Spectrometer. The investigation of the structural analysis showed the existence of $Cd(OH)_2$, mixed $Cd(OH)_2$/CdO and CdO nanoparticles. The optical absorption wavelength at 294nm in UV-Vis spectra confirmed that the reduction of Cd^{2+} ions. FTIR spectra display the vibrational modes of *veldt grape leaf* extract involved in chemical bonding and reductions. From EDAX spectrum confirmed the presence of Cd and O elements in the prepared samples. SEM and TEM images revealed nanorods, platelet and spherical shape morphologies with particle size ranging from 5.7 to 29nm. The photocatalytic activity of prepared nanoparticles was tested by degrading anionic and cationic dyes like *congo red, methyl orange* and *crystal violet* under UV-light irradiation. As well as antimicrobial activity was evaluated against gram-positive *staphylococcus aureus*, gram-negative *proteus vulgaris* and fungal- *aspergillus niger*. Comparing these three products CdO NPs exhibit high performance on both microbial and photocatalytic activity without a secondary product. Thus, the prepared CdO nanoparticles may further use in sewage treatment and biomedical applications.

OP-33

Transfer Learning-Driven Prediction of Dielectric Properties in PVDF-rGO Composites for Advanced Material Applications

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Abstract:

The integration of transfer learning into material science enables accurate property predictions for composite materials, even with limited datasets. This study utilizes a pre-trained machine learning model, fine-tuned with a PVDF-rGO composite dataset, to predict key dielectric properties such as dielectric constant and loss. By adapting knowledge from a broader dataset of materials with analogous structural and electrical characteristics, the model establishes robust correlations between parameters like band gap, phonon frequencies, and density. This approach not only enhances predictive accuracy but also accelerates the design of high-performance composites for applications in flexible electronics, sensors, and energy storage. The work demonstrates the potential of transfer learning to revolutionize material discovery and optimization.

Keywords: Transfer learning, PVDF-rGO composites, Dielectric properties, Composite materials

OP-34

Magnetic nanoparticles of Fe_3O_4 biosynthesis using *Anacardium occidentale* fruit extract: Evaluation of *in vitro* antioxidant, antibacterial, antidiabetic, anti-cholinergic and cytotoxic activities

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Abstract

The novelty of this study is to present a green method for the synthesis of Fe_3O_4 nanoparticles (Fe_3O_4NPs) using the extract of *Anacardium occidentale*. Fe_3O_4NPs were synthesized by a simple, cost-effective and environmentally friendly method. Various spectroscopic techniques confirmed the successful synthesis of Fe_3O_4NPs. UV-Vis spectrum analysis confirmed the synthesis of Fe_3O_4NPs at absorption of 310 nm. FTIR analysis confirmed the presence of several important functional groups and XRD analysis showed that Fe_3O_4NPs have a crystalline structure. FESEM and HR-TEM analyses showed that the particles have a spherical shape with a size of 19.33 nm. Furthermore, Fe_3O_4NPs indicate that they have excellent antioxidant activity of DPPH (64.92 ± 1.17%) and ABTS (73.67 ± 1.13%). In antibacterial activity, Fe_3O_4NPs exhibited the highest ZOI against *Escherichia coli* (24.58 ± 1.29 mm) and *Staphylococcus aureus* (23.74 ± 1.24 mm). At a concentration of 100 mg/mL, Fe_3O_4NPs showed the most anti-inflammatory activity against COX-1 (70.35 ± 0.89) and COX-2 (76.48 ± 0.93). In addition, Fe_3O_4NPs exhibited excellent enzymatic inhibitory activity of α-amylase (63.47 ± 0.97%) and α-glucosidase (70.58 ± 1.14%). The anti-cholinergic activity of Fe_3O_4NPs was demonstrated by the enzyme inhibition of AChE (76.19 ± 1.10%) and BuChE (84.91 ± 1.14%). Cytotoxicity study showed that Fe_3O_4NPs at 100 µg/mL significantly reduced cell viability (24.78 ± 0.56%) of HepG2 liver cancer cells. Molecular docking studies confirm that strong binding affinity to AChE and BuChE proteins. Overall, the results of this study show that the synthesized Fe_3O_4NPs have considerable efficacy for various biological applications.

Keywords: *Anacardium occidentale*, Antioxidant, Antibacterial, Anticancer, Molecular docking

DAY 2 - 04.02.2025

ORAL SESSION-III

10.35 AM to 11.35 AM,

Venue: Central Seminar Hall

OP-35

Effect of Composition on UV Filtering Nature of PVA-Bi_2O_3 Nanocomposite Films

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Abstract:

Bismuth oxide (Bi_2O_3) is a promising material for various applications due to its high attenuating nature, wide bandgap, non-toxicity, electrical conductivity and stability. In present work its UV filter capability was studied for different grain sizes in PVA matrix using 352nm UV light source. The Ultraviolet filtering capability was measured using custom made experimental setup equipped a dedicated source meter which interfaced with photodiode. In prior, pencil hardness test was carried out to ensure its hardness. Our experimental finding confirms Nano Bi_2O_3 nanocomposite exhibits higher UV filtering capability compared to it's bulk and also higher composition composite film as high UV filtering capability due to the higher surface-to-volume ratios and multiple scattering processes. These results will be discussed with suitable mechanism.

Keywords: *Bismuth Oxide; UV filter; Pencil hardness test; Grain size effect; Composition effect;*

OP-36

Poly(vinyl)pyrrolidone - an additive for zinc phosphate coating

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Department of Chemistry, CEG Campus, Anna University, Chennai.

Abstract:

Finding new additives for coatings to protect the surfaces is always receives attention. This study explores the enhancement of corrosion resistance in mild steel through the application of poly(vinyl pyrrolidone) (PVP) incorporated zinc phosphate coating. A thorough analysis of the newly formed coatings revealed that the PVP had contributed significantly in the formation of well-defined coating with reduced cracks and improved crystal density. Besides, the added PVP reduced the dissolved iron content and the hydrophilicity of the steel substrate. The corrosion resistance of the coatings was assessed in both neutral (3.5% NaCl) and acidic (0.5M HCl) aqueous environments using potentiodynamic polarization and electrochemical impedance techniques. The findings revealed that the inclusion of PVP in the phosphating bath proficiently enhanced the corrosion resistance of the coating exposed to the neutral medium, underscoring its potential utility in corrosion prevention strategies for mild steel used in this environmental condition.

OP-37

Study on the extent of degradation of Chlorpyrifos pesticide using biosurfactant-producing bacterial strains isolated from agricultural soil

Sanchali Bose, Dr. P. Senthil Kumar, Dr. B. Chitra,

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Abstract

Pesticide can create an imbalance of the ecosystem and can negatively impact human health if being used in unregulated quantities. Thus, remediation of the persistent pesticides poses an important step to protect human lives and the environment. The conventional methods of pesticide degradation have been found to be not highly efficient in removal. In this paper, it is intended to understand how the potential of biosurfactant producing microbes can be used to degrade a widely used organophosphorus pesticide named chlorpyrifos. 5 isolates which could tolerate chlorpyrifos were further tested for biosurfactant production via parafilm test, oil spreading test, and emulsification index test. 2 isolates were positive for all the tests and were considered to be producing biosurfactants. Upon subjection to FTIR, it was further confirmed that the produced biosurfactants are lipopeptides in nature. The confirmed strains upon identification through 16srRNA, was confirmed to be Bacillus cereus strain DIF1 and Bacillus cereus strain INACH001. UV Spectroscopy identified that the strains could efficiently degrade chlorpyrifos completely till 150 ppm in a time span of 7 days at 6.5 pH and at 30°C. The supernatant of the aqueous sample extracted from the degradation experiments were subjected to GCMS for metabolite studies. For Bacillus cereus strain DIF1, the metabolites present were 2-Chloroethyl methyl sulfoxide and Dichloroacetaldehyde while for Bacillus cereus strain INACH001 the detected metabolites were Methylene chloride and Carbonic chloride fluoride. Finally, it could be concluded that the above-mentioned lipopeptide producing strains could completely remediate chlorpyrifos upto a considerable concentration.

OP-38

Hybrid Nanocomposite as a Photocatalyst for Enhanced Hydrogen Production under Direct Solar Light Radiation

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Abstract

The present work focused on the synthesis, characterization and photocatalytic performance of CuO/Cu_2O loaded YVO_4 for hydrogen production under solar light irradiation. YVO_4 and CuO nanoparticles were synthesized using the hydrothermal method, with CuO impregnated on YVO_4 via wet impregnation. XPS analysis revealed the presence of Cu^+ and Cu^{2+} in the nanocomposite, while XRD identified CuO as the primary phase. The reduction of CuO to Cu_2O occurred through in-situ chemical reduction by CO, possibly released from surface organic compounds on YVO_4 during calcination. The resulting $CuO/Cu_2O/YVO_4$ nanocomposite formed a p-n heterojunction at the Cu_2O/YVO_4 interface, following an S-scheme mechanism between Cu_2O as the reduction photocatalyst (RP) and YVO_4 as the oxidation photocatalyst (OP). Additionally, the CuO/Cu_2O bilayer heterojunction facilitated a Z-scheme mechanism for interfacial charge transfer, significantly suppressing electron-hole recombination, as confirmed by photoluminescence spectra. XRD analysis indicated a lower angle shift in peaks, suggesting Cu^{2+}/Cu^+ ion substitution for V^{5+} ions in YVO_4 and lattice compression due to oxygen vacancies. DRS-UV-Vis spectra exhibited a red shift attributed to impurity energy levels at heterojunctions. The more negative reduction potential of Cu_2O enhanced the hydrogen evolution rate (HER). Consequently, the optimized 0.7 wt% $CuO/Cu_2O/YVO_4$ nanocomposite achieved a hydrogen production rate of 6.25 mmol h^{-1} g^{-1}, outperforming pristine YVO_4 (3.75 mmol h^{-1} g^{-1}). This work highlights the effective synergy of S- and Z-scheme mechanisms in $CuO/Cu_2O/YVO_4$ for improved photocatalytic hydrogen production.

OP-39

Enhanced photocatalytic degradation using Sulfur-doped TiO_2/g-C_3N_4 composite

Jeny Rachel Biju[a], Jacklien Emema Rose T.J[a], Jason Thamizhakaran Stanley[a], Amudha Thanarasu[b], Sathya Selva Bala Vasantha Kumar[c] Baskaralingam Palanichamy[d], Sivanesan Subramanian[a]*

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Abstract

The effective elimination of organic contaminants from water persists to be a major concern for environmental sustainability. This work investigates how sulphur doping improves the photocatalytic performance of TiO_2/g-C_3N_4 composite photocatalysts for organic pollutant degradation under visible light irradiation. Incorporating sulphur into TiO_2 optimises its electrical characteristics and extends its absorption into the visible region, improving photocatalytic activity in a Z-scheme system. The S-TiO_2/g-C_3N_4 composite was synthesised using a simple, cost-effective approach and characterised using several methods, including XRD, SEM, UV-DRS. The effect of sulphur doping on photocatalytic activity has been evaluated using organic dye degradation tests under visible light. Sulphur doping greatly improves photocatalytic performance of TiO_2/g-C_3N_4 composites. The modified composite degraded pollutants more quickly, which was due to better charge carrier separation and the development of defect states that facilitate electron transfer. While sulphur doping reduces the bandgap of TiO_2, the Z-scheme heterojunction between TiO_2 and g-C_3N_4 enables effective charge separation. This study emphasises the significance of sulphur doping and defect engineering to improve the photocatalytic abilities of TiO_2/g-C_3N_4 composites. These composites are potential prospects for effective environmental remediation due to their improved charge separation and farther light absorption.

OP-40

Monoclinic $BiVO_4$ Nanosphere for High Performance Supercapacitor

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Abstract

A facile and cost-effective strategy was employed to synthesize cobalt-doped bismuth vanadate (Co- doped BiVO4) nanoparticles (NPs) using a one-step hydrothermal method. The synthesis was conducted at 180°Cover 24 hours. The synthesized Co- doped BiVO4 NPs were characterized using X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), high-resolution transmission electron microscopy (HR-TEM), X-ray photoelectron spectroscopy (XPS), and electrochemical analyses. The XRD patterns revealed a combined monoclinic crystal structure. FE-SEM and HR-TEM images clearly demonstrated the formation of nanospheres and needle-like structures in the cobalt-doped BiVO4. Electrochemical studies showed that Co- doped BiVO4 exhibited enhanced specific capacitance, attributed to the optimized nanostructure. The material achieved a high specific capacitance of 424.8 F g^{-1} at a current density of 1 A g^{-1}, retaining 81.13% capacitance after 5,000 cycles at 10 A g^{-1} in a three-electrode system, and 88.18% after 10,000 cycles in a two-electrode system. This work demonstrates the potential of transition metal vanadate, such as cobalt-doped BiVO4, as promising electrode materials for next-generation energy storage devices, with low toxicity and reduced environmental impact.

OP-41

The Evolution of 2D Core@Shell Nanoarchitecture for Supercapacitor Application

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Abstract

Supercapacitors can store energy for use in portable devices, electric vehicles (EVs), and renewable energy systems. These topologies support quick charge-discharge cycles, making them ideal for high-power applications such as regenerative braking in EVs and hybrid energy systems. The gradual improvement of these nanostructures, where core materials and shell coatings are designed to attain advanced features for a variety of applications, is known as the evolution of 2D core@shell nanoarchitecture. Innovation in core and shell materials, multilayer and heterostructure designs, and other areas are all part of it. The 2D core@shell nanomaterial fabrication focusses on producing innovative materials such as transition metal oxides and dichalcogenides, optimising shell thickness, and constructing hybrid systems that combine supercapacitors and batteries. The core@shell nanoarchitecture dates back to early 1990s and with its significance around 2000s with the development of materials like graphene. By around 2010 In the areas of material selection and design, synthesis techniques, and functionalization, 2D core@shell nanoarchitectures saw improvements and breakthroughs. Improving electrolyte compatibility and stability are other important areas of investigation. The benefits include increased surface area, increased energy density, faster charge-discharge cycles, and higher mechanical stability. However, issues like as complicated synthesis, material compatibility, scalability, and long-term stability exist. This 2D core@shell nanoarchitecture is critical for developing supercapacitors, providing enhanced energy storage capacity for current applications. Overcoming present hurdles through material and process innovation will allow for scalable, cost-effective energy solutions in the future.

DAY 2 - 04.02.2025

ORAL SESSION-IV

01.30 PM to 02.30 PM,

Venue: Central Seminar Hall

OP-42

Green Synthesis of zinc oxide nanoparticle using azadirachta indica extract for removal of pollutants from diary effluent

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Abstract

Wastewater management is a critical global challenge, and the quest for environmentally friendly and sustainable treatment methods has gained significant attention. Biosynthesis of nanoparticles as the name indicates help in the synthesis of very complex reaction within a fraction of minutes have now taken up the attention towards synthesis grievance the need of environmentally benign technologies in material science. This abstract presents a comprehensive overview of the application of green synthesis in wastewater treatment processes, focusing on its potential to provide sustainable and eco-friendly solutions. Green synthesis involves the use of natural, renewable resources and environmentally benign methods to fabricate nanomaterials with exceptional properties for water treatment. Zinc Oxide have many and very impressive properties like large binding energy, wide band gap, high piezoelectric property etc. To the best of our knowledge, the use of leaf extract Ocimum Tenuiflorum plant for green synthesis of ZnO nanoparticles has not been revealed. Hence the present task was carried out to synthesis and characterization of ZnO nanoparticles using leaves extract of Ocimum Tenuiflorum plant.This paper highlights the green synthesis method using neem extracts, in the production of zinc oxide nanoparticles. These nanoparticles exhibit unique physicochemical characteristics, such as high surface area, reactivity, and stability, making them effective for the removal of contaminants from wastewater. Additionally, the environmentally benign nature of green synthesis methods reduces the ecological footprint associated with traditional synthesis approaches. The phytochemicals present in neem are alkaloids, quinines, resins, tannins, flavanoids, fats, saponins, phenolic compounds, Proteins and carboxylic acids (Khan et al., 2010). It is important to find an alternate way for the treatment of waste water in a more sustainable and cost-effective manner.

The present study discusses the diverse applications of green-synthesized nanomaterials in wastewater treatment, including the removal of heavy metals, organic pollutants, and pathogens.

OP-43

Enhancing the Performance of Hybrid Perovskite Solar Cells through Additive Engineering

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Abstract

Hybrid perovskite solar cells (HPSCs) have garnered significant attention due to their high-power conversion efficiencies, low production costs, and tunable optoelectronic properties. Despite these advantages, challenges such as long-term stability, phase instability, and non-radiative recombination hinder their commercial viability. Additive engineering has emerged as a promising strategy to address these issues by tailoring the material properties at the molecular level. This study explores the incorporation of various additives, including organic and inorganic salts, into the perovskite precursor solution to optimize crystal growth, reduce defect density, and enhance charge transport. The effect of different additive concentrations on the perovskite film morphology, optical properties, and photovoltaic performance is systematically analyzed. Devices fabricated with optimized additive concentrations demonstrate improved phase purity, increased carrier lifetime, and enhanced stability under environmental stress conditions. These findings underscore the critical role of additive engineering in advancing the performance and scalability of HPSCs, paving the way for their deployment in next-generation photovoltaic technologies.

Keywords: Hybrid perovskite solar cells, additive engineering, defect passivation, photovoltaic performance, next-generation photovoltaics.

OP-44

Study on Corrosion Resistance Of Mild Steel By Graphene Oxide Aided Zinc Phosphate Conversion Coating

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Abstract:

Zinc phosphate conversion coatings have been successfully used as a primer coating on steels because they increase the corrosion resistance and also enhance good adhesion of the paint on substrate. The corrosion resistance of zinc phosphate conversion coating with and without Graphene oxide was studied. The main ingredients in the phosphating bath were H_3PO_4, ZnO, $NaNO_3$ and Graphene oxide. Graphene oxide (GO) is used as additive in zinc phosphating process on steel. Addition of different concentration of GO to the formulated phosphating bath were used for coating mild steel. The effect of GO on microstructure and corrosion resistance of steel phosphate coating was investigated. The Graphene oxide is obtained from modified Hummer's method which is used as additive in zinc phosphate conversion coating. GO were characterized by FT-IR, Surface morphology and elemental composition of the GO were studied using SEM and EDAX. The coating characteristics and corrosion resistance of Graphene oxide aided coated steel panel were evaluated by SEM, EDAX, XRD, Electrochemical Impedance Spectroscopy and Potentiodynamic Polarization. Potentiodynamic Polarization measurement result shows the rate of corrosion is decreased by addition of GO due to decreases in corrosion current density (I_{Corr}) and increase in polarization resistance (R_p). High polarization resistance, lowest corrosion current density is obtained for phosphate coating with GO hence it can be used to obtain better corrosion resistance of zinc phosphate coating on mild steel.

OP-45

Photoinduced Electron-transfer from substituted benzimidazole to various nano metal oxides

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Abstract

The dynamics of photoinduced electron injection and energy transfer from benzimidazole to CuO, Fe_2O_3, WO_3 and Al_2O_3 nanoparticles has been studied by FT-IR, absorption and fluorescence spectroscopic methods. The association between nanoparticles and benzimidazole derivative was explained from both absorption and fluorescence quenching data. There is good agreement between these values of K_{app} obtained from the data of fluorescence quenching with that determined from the absorption spectral changes which highlighted the validity of the association between benzimidazole and nanoparticles. The distance between the benzimidazole derivative and nanoparticles as well as the critical energy transfer distance has been calculated.

OP-46

Phytochemical Screening of Sponge Gourd and Their Antioxidant, Antibacterial Activity

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Abstract

This study explores the phytochemical profile and antibacterial potential of *Luffa aegyptiaca* (sponge gourd) leaf extracts. The leaf material was subjected to Soxhlet extraction to isolate bioactive compounds, and the phytochemical constituents were identified through standard colorimetric methods. The extracts revealed the presence of several secondary metabolites, including cardiac glycosides, flavonoids, saponins, and tannins, which are known for their bioactive properties. To assess the antibacterial activity, the extracts were tested against two bacterial strains: *Bacillus subtilis* and *Escherichia coli*. Antibacterial efficacy was evaluated by measuring the zone of inhibition in millimeters, demonstrating significant antibacterial activity in both cases. The results suggest that *Luffa aegyptiaca* leaf extracts possess potent antibacterial properties, which could be explored for the development of natural antimicrobial agents. These findings highlight the therapeutic potential of *Luffa aegyptiaca* in combating bacterial infections and underscore the importance of further investigation into its bioactive components.

OP-47

Removal Of Chromium From Tannery Effluent Using Aged Refuse As Adsorbent

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Abstract

This study focuses on the removal of chromium from secondary treated tannery effluents using aged refuse as an adsorbent and analyzing recalcitrant characteristics, emphasizing its environmental significance and cost-efficiency. Chromium, particularly in its hexavalent form (Cr(VI)), poses severe health and ecological risks due to its high toxicity and mobility. Conventional treatment methods are expensive and generate secondary pollution, making alternative methods necessary. Aged refuse, a readily available and underutilized material in Tamil Nadu, was chemically modified with nitric acid to enhance its adsorption properties. The study involved characterizing aged refuse through techniques such as SEM, XRD, BET, and FTIR to understand its structural and functional attributes and Langmuir and Freundlich adsorption isotherm study for understanding adsorption carried out. Adsorption experiments are done to find optimized key parameters such as Temperature ,contact time, pH, and dosage to maximize chromium removal. The results will demonstrate that aged refuse could effectively reduce chromium concentration, offering a sustainable, low-cost solution for tannery wastewater treatment. This research highlights the dual benefits of waste management and environmental remediation by converting landfill material into a valuable resource for pollution control.

OP-48

Synthesis And Spectral Characterization Of Naphthalen-2-Yl-N′-(2-Hydroxybenzoyl) Benzohydrazonate Cobalt(Iii) Complex

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Abstract

New ligand naphthalen-2-yl-N′-(2-hydroxybenzoyl)benzohydrazonate (NHBH) has been prepared and characterized by IR, ^{1}H NMR, ^{13}C NMR and Mass Spectroscopic techniques. To an ethanolic solution of $CoCl_2.6H_2O$ the equimolar ligand solution was added. The reaction mixture was then refluxed for 5 h. The pink suspension gradually turned purple. The completion of the reaction and purity of the new complex was checked by TLC. The solvent was removed under reduced pressure. The new complex was characterized by various spectroscopic studies such as IR, Uv-Vis, ^{1}H-NMR and ^{13}C-NMR. The results obtained from the above spectral studies, it was inferred that the ligand coordinated to cobalt metal and resulted in a diamagnetic Cobalt(III) octahedral complex. The new complex is soluble in common organic solvents such as dichloromethane, Ethanol, methanol, dimethylformamide and dimethyl sulfoxide.

Keywords:naphthalen-2-yl-N′-(2-hydroxybenzoyl)benzohydrazonate,$CoCl_2.6H_2O$,IR spectroscopy, ^{1}H NMR spectroscopy and ^{13}C NMR spectroscopy

OP-49

Leachate treatment by using phytoremediation technique

*Mohamed Riyas Shahul Hameed[1], Jason Thamizhakaran Stanley[2], Jackline Emema Rose T.J[2], Amudha Thanarasu[3], Sathya Selva Bala Vasanthakumar[4],Sivanesan Subramanian[2] , Arulmozhi Rajendran[1]**

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Abstract

Leachate treatment is an important aspect in solid waste management and it is highly toxic liquid waste generated from landfill sites, poses significant environmental risks due to its high concentration of organic and inorganic pollutants, including heavy metals and nutrients. The transport of leachate affects the natural ecosystem and wellbeing of human life. This project investigates the potential of phytoremediation, a sustainable and eco-friendly approach for the treatment of leachate using selected plant species. The viability of phytoremediation as a cost-effective and sustainable leachate treatment strategy, offering an alternative to conventional methods. The research focuses on the ability of these plants to absorb, degrade, and detoxify pollutants from leachate. To measure the reduction in pollutant concentrations such as nitrogen, phosphorus, heavy metals, and organic compounds from leachate after treatment using phytoremediation techniques. The study includes a comprehensive analysis of the physico-chemical properties and nutrient levels. Advanced analytical techniques, including Atomic Absorption Spectroscopy (AAS) and spectrophotometric methods, are employed to quantify pollutant concentration. In this study, selected plant species exhibit potential for heavy metal uptake and also efficient in nutrient removal. An attempt has been made to investigate the removal efficiency of pollutants from leachate by phytoremediation technique.

***Keywords*:** Phytoextraction, heavy metal, nutrients removal, sustainability

OP-50

Indium-doped MoS_2 as a wearable thermoelectric generator

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Abstract

The human body produces a large amount of heat every day. It would be a giant leap for mankind if this heat energy could be converted into electrical energy by applying the concepts of thermoelectrics. Thermoelectrics is the field that establishes the relationship between heat and electrical energy using the Seebeck effect. Since this technique doesn't depend on external factors like sunlight, it has a cutting edge over the other models. The usage of transition metal dichalcogenide, MoS_2 for this purpose will be effective due to its scalability, thickness-dependent electrical properties, attractive electronic and optoelectronic properties such as valley degeneracy, large effective mass, and anisotropic properties. In this work, we studied the concentration influence of indium doping in MoS_2 on the Seebeck coefficient, and thereby on the material's electrical conductivity. Various concentrations of In-MoS_2 were prepared using a facile hydrothermal method on functionalized carbon fabric. Basic material characterization was done to confirm the crystal structure, phase purity, and morphology. Characteristics such as the Seebeck coefficient, Electrical conductivity, and Hall measurement are being studied to validate the potential application of In-MoS_2 in thermoelectric generations.

OP-51

A Computational Study on ZrPdCC Half-Hesuler Alloys For Thermoelectric Applications

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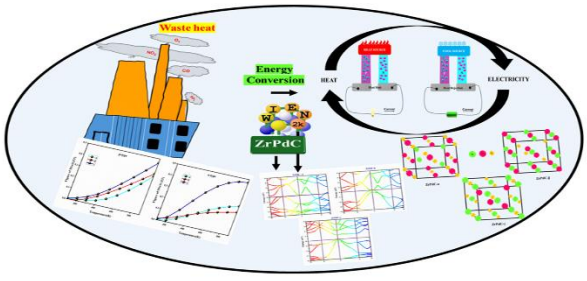
Abstract:

In this work, we performed a detailed computational study on the structural, mechanical, electrical, and thermoelectric properties of half-Heusler alloy ZrPdC, which were investigated using Density Functional Theory (DFT). The structural characteristics and electronic properties of ZrPdC alloy are computed using the generalized gradient approximation (GGA-PBE). Based on calculations of the density of states and electronic band structures, it has been assumed that the half-Heusler alloys behave as metal in α-phase, pseudo-metal in β-phase, and semiconductor in γ-phase with direct bandgaps. The mechanical properties are computed using the IR-elast code, indicating the material stability. Furthermore, the thermoelectric properties such as the Seebeck coefficient, power factor, thermal and electrical conductivity, and figure of merit (ZT) were estimated at different temperatures by combining DFT calculations with semi-classical Boltzmann transport theory. The value of Seebeck coefficient for n-type α-ZrPdC, β-ZrPdC and γ-ZrPdC are -85.90 μV/K, -23.70 μV/K, and -60.26 μV/K, respectively at 900K and the corresponding power factor is $129x10^{-3}$W/mK^2, $34x10^{-3}$W/mK^2, and $77x10^{-3}$W/mK^2 at the same temperature. Therefore, the maximum ZT observed for γ -ZrPdC is about 0.4 at 900 K, while for α-ZrPdC and β-ZrPdC it is about 0.3 and 0.2 at the same temperature. Due to their thermoelectric properties, these alloys are suitable for applications in thermoelectric energy devices.



OP-52

Computational Insights and Molecular Docking of Zalcitabine on Noble Metal-Loaded Silica Nanocomposites: A Novel Approach for COVID-19 Therapeutics

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Abstract:

The rapid evolution of the COVID-19 pandemic necessitates innovative drug discovery strategies. Utilizing existing medications and evaluating commercially available inhibitors against the virus's targets offers a promising approach. This research explores the characteristics and adsorption behavior of Zalcitabine (ZAL) on silica nanocomposites loaded with noble metals (Au/Ag/Pt), employing quantum chemical calculations based on the density functional theory (DFT). The optimized geometry of the molecule was determined via the DFT/B3LYP method with the LANL2DZ basis set. Electronic absorption spectra for ZAL and its complexes were analyzed using TD-DFT in various solvents, including polar protic and aprotic types. Charge transfer mechanisms were investigated through the energy levels of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). A molecular electrostatic potential map visualized charge distribution using a color-coded scheme. Druglikeness and lipophilicity properties were assessed to evaluate ZAL's potential for drug delivery. Finally, molecular docking studies with selected proteins were performed for both the ligand and its complexes, providing valuable insights into their therapeutic potential.

Keywords: Zalcitabine; COVID-19; DFT; Molecular docking; Nanocomposites

DAY 1 - 03.02.2025

POSTER SESSION - I

(4.15 PM to 5.30 PM)

Venue: Main Auditorium

PP-01

Review on Advanced Hybrid Nanomaterials Including 2D Materials for High Performance Supercapacitor Applications

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2. Associate Professor, Department of Physics, SRM Institute of Science & Technology, Tiruchirappalli- 621 105, Tamil Nadu, India.

Abstract

The increasing demand for efficient and sustainable energy storage solutions has sparked considerable interest in two-dimensional (2D) materials for supercapacitor applications. Present research workcould explore the creation of hybrid materials that combine molybdenum disulfide (MoS_2), rhenium disulfide (ReS_2), and reduced graphene oxide (RGO) as electrode materials. Those hybrids could produce using a hydrothermal method and characterization is to be done through X-ray diffraction (XRD) and Raman spectroscopy to verify their structural and compositional characteristics. The interaction between the species at electrode surface and electrolyte enhancing their electrochemical properties, with MoS_2 and ReS_2 would contribute high pseudocapacitance while the inclusion of RGO and further turn up very high electrical conductivity and stability. Electrochemical assessments, including cyclic voltammetry and charge-discharge tests may reveal high specific capacitance, impressive energy and power densities, and outstanding cycling stability. Present study expected to empower the potential of 2D hybrid nanomaterials as promising species for next-generation supercapacitors, meeting the increasing demand for reliable and efficient energy storage solutions in contemporary technologies.

PP-02

Environmental Friendly Materials

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Abstract

The progress in biodegradable plastics is crucial for addressing the growing environmental challenges associated with traditional plastics. Unlike their conventional counterparts, which can persist in the environment for centuries, biodegradable plastics are designed to decompose more swiftly under natural conditions. This attribute substantially reduces plastic waste pollution. Such materials can be classified into several categories: those derived from plants (e.g., PLA, PHA), those based on petroleum (e.g., PBAT, PBS) and hybrid materials. Thus, this diversity offers numerous options for various applications. The raw materials used encompass renewable resources like corn, sugarcane, algae and even waste-derived inputs (e.g., food or agricultural byproducts). The manufacturing process of biodegradable plastics involves polymerization techniques and emerging technologies are focusing on improving efficiency and performance. The degradation mechanisms include microbial action, enzymatic breakdown and environmental factors, such as moisture and temperature. These plastics serve multiple purposes in packaging, agriculture and the medical sectors, however, their widespread adoption still faces challenges.

Challenges, however, persist; notably, high production costs, limited performance and a lack of adequate recycling infrastructure remain formidable obstacles in the widespread adoption of biodegradable plastics. The environmental advantages of these materials are considerable, providing significant reductions in plastic pollution (and) supporting compostability, which can enhance soil health. A strong regulatory framework—such as standards like ASTM and ISO—is crucial for ensuring their effectiveness. Recent innovations focus on bio-based materials, marine biodegradability and the integration into circular economies. Although challenges continue, continued research, public awareness and consumer education are vital for advancing the widespread adoption of biodegradable plastics as a sustainable alternative to conventional plastic products because this transition is essential for environmental sustainability.

PP-03

Synthesis And Characterization of Gallic Acid Functionalized Biomagnetic Hydroxyapatite/Alginate Hydrogel Beads Bio-Nanocomposite For Biomedical Applications.

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Abstract

This study presents the synthesis and characterization of Hydroxyapatite (HAp)-Fe_3O_4 -Gallic Acid hydrogel beads on alginate biopolymer, a novel nanocomposite designed for potential biomedical and drug delivery applications. The HAp-Fe_3O_4-Alginate-Gallic acid nanocomposite was fabricated by a simple method, aiming to combine the biocompatibility and bioactivity of hydroxyapatite with the magnetic properties of Fe_3O_4 and the antioxidant potential of gallic acid, based on ionotropic gelation of alginate matrix. The morphology and particle size of the hydrogel beads were analyzed by Scanning Electron Microscopy (SEM), which showed well-distributed particles with a uniform surface around 9-25 nm. The elemental composition was confirmed by Energy Dispersive X-ray Spectroscopy (EDX), which revealed the presence of calcium (Ca), phosphorus (P), iron (Fe), and carbon (C), affirming the successful incorporation of Fe_3O_4 into the HAp-alginate matrix of the beads. The magnetic properties of the Fe_3O_4 and the nanocomposite were investigated using Vibrating Sample Magnetometry (VSM), which demonstrated strong coerocivity and retentivity, making the nanocomposite suitable for targeted drug delivery and magnetic assisted therapies. Fourier Transform Infrared Spectroscopy (FTIR) analysis confirmed the functional groups associated with HAp, Fe_3O_4, alginate, and gallic acid, indicating the successful integration of the nanocomposite. The incorporated hydrogel beads showed strong anti-bacterial activity against *S.aureus* and *E.coli*. The results indicate that this nanocomposite holds significant promise for biomedical applications, particularly in drug delivery, tissue engineering, and as a therapeutic agent due to its magnetic, antioxidant, and bioactive properties.

Keywords: Hydroxyapatite; Fe_3O_4; Alginate matrix; Anti-bacterial activity;

PP-04

Green synthesis of AgNPs using *Albizia Saman Gum*-natural biopolymer: Evaluation of its Antibacterial and Catalytic activity

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Abstract

In this study, AgNPs were synthesized using *Albizia Saman gum* extract which act as a capping agent and also as reducing agent. The synthesized AgNPs using *Albizia Saman gum* extract was characterized by analytical techniques which are Ultraviolet-Visible (UV-Vis) spectroscopy, Fourier Transform Infrared (FTIR) spectroscopy, Energy Dispersive X-Ray spectroscopy (EDS), X-Ray Diffraction (XRD), Scanning Electron Microscope (SEM). The UV-Spectra showed the absorption band at 420 nm. This absorption peak indicating that the Silver Nitrate ($AgNO_3$) solution was reduced to silver nanoparticles (AgNPs). FTIR indicated that the functional groups like C=O, O-H, C=C were present in the synthesized GABS-AgNPs. The presence of Ag in the synthesized AgNPs was clearly indicated in EDS Spectra and some of the trace elements like C, O, etc. are also present in the synthesized nanoparticles. Surface morphology of synthesized AgNPs was studied in the SEM, it stated that it is spherical in shape with the average 90nm in size. The XRD study point out that the particles are crystalline in nature, with a face centered cubic (FCC) structure. The Catalytic degradation of 4-Nitrophenol was evaluated using AgNPs. The 4-Nitrophenol was reduced to 4-aminophenol in the presence of $NaBH_4$. The antibacterial activity of synthesized GABS-AgNPs was very good effective (Inhibition Zone – 5mm & 3mm) against *E. coli and S. aureus bacteria.*

Keywords: AgNPs, Albizia Saman, Anti-Microbial Activity.

PP-05

Enhancing the Catalytic Potential of Sm and Sm@Ag-Doped Strontium Titanate for Sustainable Energy and Environmental Applications

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Abstract

The Sm and Ag doped $SrTiO_3$ nanoparticles have been effectively produced by using a sol-gel method with citric acid acting as a chelating agent in the ethylene glycol solution for the efficient photodegradation of methylene blue dye under visible light irradiation. All samples show evidence of the creation of the cubic perovskite structure according to X-ray diffraction (XRD) analysis. Images captured by field emission scanning electron microscopy (FESEM) have verified that the addition of doping elements has reduced the particle size and ensured consistency in the samples. The produced samples' UV-vis spectra show a blue-shift in the absorption tail as well as a decrease in band gap energies of 3.61 eV, 3.56 eV, and 3.53 eV with $SrTiO_3$, $Sm@SrTiO_3$, and $Sm@Ag@SrTiO_3$. The ideal photocatalyst operating conditions were determined to be 5 ppm of initial Methylene Blue (MB) concentration, 0.005 g/L of catalyst dosage, and 100 minutes of irradiation time. Additionally, the photocatalytic analysis shows that the doped sample has a higher rate of MB degradation under visible light. $Sm@Ag@SrTiO_3$ nanoparticles exhibit 80% higher photocatalytic activity compared to $Sm@SrTiO_3$ and $SrTiO_3$, which have efficiencies of 50.88% and 30.23%, respectively. The trans-esterification process was optimized using a 4:1 alcohol-to-oil molar ratio, 100 mg of $Sm@Ag@SrTiO_3$ NPs catalyst, a 60-minute reaction time, and 80 °C temperature, achieving a biodiesel yield of up to 85%. The catalyst maintained high efficiency over multiple runs, demonstrating consistent performance and stability. These findings emphasize the catalyst's potential for cost-effective and sustainable biodiesel production.

Keywords: Visible light; Methylene blue; $SrTiO_3$; Biodiesel;

PP-06

Polyimide Composite and Polymer Encapsulant Material for Spacecraft Electronic Packages

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Abstract

The space program and development in space research has been prime focus of many developed and developing countries. It provides the country with a broad scope of beneficial applications which includes citizen development, mass communication, agriculture, economy, defence, scientific and medical research . Satellite, Launch Vehicle and Space Centre are the three key components under the umbrella of any space program. Modern society has evolved to include a wide range of electronic devices and equipment, all of which have components made of electronic materials. Polymers and polymer composites, essential for modern civilisation, offer low-density, durable solutions for advanced electronics operating at higher temperatures. As it covers synthetic polymers, bio polymers, polymer characterisation, product design and production for a safer and more sustainable environment, polymer science is an interdisciplinary field. Polymer materials are widely used in electronics for their lightweight, high strength, dimensional stability, low thermal expansion, and superior fatigue and fracture resistance. Composite materials, particularly polymer composites, have revolutionised spacecraft electronics with their multifunctional, adaptable properties suitable for extreme space environments. This paper also efforts to review the potential uses of Composite materials in Space industry. This paper also emphasizes the importance of polymer composites and polymeric encapsulants used for spacecraft electronics and their properties are characterized for usage in space program.

PP-07

Optimized Photocatalytic Breakdown of Rhodamine B Dye Using Iron Titanate (Fe_2TiO_5) Nanoparticles Synthesized Via A Modified Sol-Gel Process

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Abstract

In this work, modified sol- gel technique was employed using the interaction of the solutions of binary nanoparticles Fe_2O_3 and TiO_2 the synthesis of iron titanate (Fe_2TiO_5) nanoparticles and a potential photocatalyst candidate for photocatalytic and various other applications. The photocatalytic activity of prepared Fe_2TiO_5 nanoparticles was evaluated by the degradation of cationic dye-Rhodamine B. The adsorption capacity and photocatalytic activity in the process of decolourization of the rhodamine B dye (RhB) was investigated in an extensive manner. All diffraction peaks can be indexed to the orthorhombic phase of Fe_2TiO_5 nanoparticles. The shape of the nitrogen isotherm could be considered to be a type V isotherm which is typical for mesoporous materials. Direct and indirect band gap values were estimated as 2.16 and 1.81 eV, respectively. Fe_2TiO_5 powder consisted of relatively uniformly sized nanoparticles with a rhombic shape ranging from 28 to 83 nm. The peaks originating from Fe_2TiO_5, at approximately 425 and 800 cm^{-1} representing vibrations of Fe–O and Ti–O bonds. Photoluminescence spectrum of Fe_2TiO_5 nanoparticle powder measured with an excitation wavelength of 270nm.The following supporting studies like P-XRD, N_2 adsorption-desorption isotherms, UV-vis-DRS, FTIR, FE-SEM and Photoluminescence techniques were adapted in the analysis of structural, optical and surface morphological property of the synthesized catalyst.

Keywords: Photocatalytic activity, Rhodamine B dye, Iron titanate, Sol-gel method, Band gap.

PP-08

In Vitro Characterization of Clay Nanotube Formulations For Dermatological Applications

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Abstract

This study presents an in vitro analysis of clay nanotube-based combinations for dermatological applications, where the advantageous properties of clay nanotubes are used to provide controlled delivery of active substances as they are inexpensive and widely available. The study intends to look into the sun protection factor (SPF) of the formulations, their anti-hyperpigmentation and moisturizing abilities. The determination of SPF and the inhibition of hyaluronidase were carried out via UV-Visible spectrophotometry, while the inhibition of tyrosinase was done to evaluate the formulation's ability to suppress melanin. The results showed that the SPF was 9.5, while the inhibition rates of tyrosinase and hyaluronidase were found to be 46.82% and 62.56%, respectively, which proved the ability of the formulation to offer UV protection and inhibit enzymes concurrently. Clay nanotubes, therefore, appear to be viable nanomaterials for use in cosmetics given the fact that they can help solve dermatological problems without the need for testing on animals and humans, which is more cost-effective and ethical. The strategy is compatible with biotechnological, ethical, and economic objectives and therefore enhances the scope for using clay nanotubes in developing skin care products.

PP-09

Purification of Metallurgical-Grade Silicon via the Acid Leaching and Roasting Method

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Abstract

The silicon kerf, also called Waste Silicon Kerf (WSK), is made by a diamond wire saw machine. The WSK contains metallic impurities from the cutting and growing processes. The average particle size of the DWSSP was first determined to be 1.8 μm. X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), field emission scanning electron microscopy (FESEM), and inductively coupled plasma mass spectrometry (ICP-MS) analysis were used to investigate the roasting method. Elemental analysis (EDS) revealed the presence of silicon (Si) at 61.3% weight percentage, oxygen (O) at 14.2%, carbon (C) at 15.8%, and other elements. Iron (Fe) and aluminum (Al), two metal contaminants, were detected in the produced sample at quantities of 580 and 367 parts per billion (ppb), respectively. The morphology and composition of WSK are systematically examined in this study, and an optimized impurity removal method combining mixed acid leaching and low-temperature oxidative roasting is suggested. This method takes advantage of the ability to remove the oxide SiO2 layer and metal impurities using HF etchant. The impact of time, acid leaching temperature, and HF concentration on the rate of impurity leaching is investigated. HF concentration of 4 mol·L−1, leaching temperature of 70 °C, and a 2-hour duration are the ideal parameters for mixed-acid leaching. Fe and the other contaminants are removed at a rate better than 99%. The recovery of silicon resources from WSK depends on this straightforward technique.

Keywords: Silicon kerf loss, Silicon recovery, Acid leaching, Impurities removal, Photovoltaic applications.

PP-10

Optimization of Hydrofluoric Acid Etching Parameters for Effective Removal of Oxygen and Metal Impurities from Silicon Kerf Loss

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Abstract

Silicon kerf loss (SKL) from diamond wire sawing in the wafering process is a highly appealing source material for photovoltaic (PV), supercapacitors, batteries, water splitting and other applications. Here, more than 50% SiO_2 presence in the silicon kerf loss. Metal purification techniques are needed to remove impurities to recover and regenerate silicon resources from diamond wire saw powder which was considered industrial waste. The dissolving process and occurrence status of the metallic impurities in SKL are unreliable. In this study, the unique and simplest etching process involves the HF acid leaching process. The optimized parameters such as acid concentration, time, liquid-to-solid ratio, and solvent rate are involved in removing the native SiO_2 layer and metal impurities from the SKL. The sensitivity sequences of precipitates to each etchant were obtained by revealing the micro-structural evolution of SKL before and after etching. Among the leaching parameters, the acid concentration of 5 mol^{-1}, liquid-to-solid ratio of 100:4 ml/g, the time at 60 min, and solvent rate of 5ml effectively reduce the oxide layer and hidden metal impurities removed from the SKL. This optimized parameter could effectively remove more than 92.96% of the SKL's oxide layer.

Keywords: Silicon kerf loss, Hydrofluoric acid, Recycling, Purification, Photovoltaic application

PP-11

Analysis of Ancient Potteries from Keeladi, Tamil Nadu, Using FTIR, XRD, and XRF Techniques

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Abstract:

A combination of Fourier-transform infrared spectroscopy (FTIR), powder X-ray diffraction (XRD), and X-ray fluorescence spectroscopy (XRF) was employed to analyse the clay fractions of pottery excavated from Keeladi, a Sangam-period urban settlement on the banks of the Vaigai River, Tamil Nadu, India. The study aimed to identify the types of clay used in pottery production and to explore the social and cultural aspects of the region. The results indicate a preference for locally available clays across the analysed sites, suggesting localized pottery production with limited exchange of ceramics between settlements. Insights from this study also contribute to understanding the organic residues found in the pottery matrix, shedding light on their potential origins and uses in ancient Keeladi society.

Keywords: FT-IR, XRD, XRF, Organic residues

PP-12

Wearable Cu-doped Ag_2S thermoelectric material as a human heat energy harvester

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Abstract

Numerous natural sources, such as solar radiation, geothermal, industrial operations, vehicle emissions, human body heat, etc., provide an abundance of heat. Nevertheless, despite their abundance, these heat sources are often ignored, and their potential uses are still untapped. Thermoelectric (TE) technology uses the Seebeck phenomenon to transform unused thermal energy into electrical energy. The TE figure-of-merit **($\mathbf{zT = \frac{s^2\sigma}{k}T}$)** has a significant impact on the performance of TE materials. A well-known and thoroughly studied class of TE materials are metal chalcogenides, particularly silver sulfide (Ag_2S). Compared to the current Bi_2Te_3 and $Mg_3(BiSb)_2$-based thermoelectric materials, Ag_2S is the first flexible inorganic semiconducting material with good mechanical behaviour like ductility and satisfactory thermoelectric performance at room temperature (RT). At RT, the electrical conductivity of commercially available Bi_2Te_3 is higher than that of the ductile Ag_2S. The TE conversion efficiency of Ag_2S may be greatly increased by doping; however, real-world applications are still far off. Therefore, the need for high-quality TE material is essential. We thoroughly examined and anticipated the structural stability, mechanical, electrical, and TE properties both experimentally and theoretically for Cu-doped Ag_2S. Therefore, the Ag_2S TE device can be utilized as a self-powered system in bluetooth, earphones, smartwatches, and as multipurpose sensors.

PP-13

Probable Interaction of Protein Z Dependent Protease Inhibitor with Plasma Pre-kallikrein as Revealed by Computational Analysis

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Abstract

Background: Blood coagulation is a complex biological process involving extrinsic, intrinsic and common phase. Protein Z Dependent Protease Inhibitor (ZPI), being a member of serpin super family, inhibits FXIa without the presence of procoagulants such as PZ, Calcium and Lipid membrane. Unlike other coagulation protease FXI is a vitamin-k independent coagulation protein. FXI polypeptide is organised into four 90-91 amino acid repeats called apple domains designated as A1 to A4 from the N-terminus and a C-terminal protease domain. The plasma pre-kallikrein (PK), the precursor of protease plasma kallikrein (PKa) is the only other protein known to share this particular configuration. Also, the gene F11 that codes for FXI is duplicated from the gene KLKB1 that codes for PK.Aim: We propose that ZPI might interact with PK as it is a FXI homolog and the gene (F11) codes for FXI and PK are orthologs. The current study is therefore aimed to probe the interaction between ZPI and PK. Methods: Genome analyses of evolutionarily significant organisms, multiple sequence alignment analyses, phylogenetic tree construction, synteny analyses and molecular docking were used for the current study.Results: It was observed that Zebra fish genome consists of two genes homologous to KLKB1 in chromosome number 12 and 14. The pattern of branching in the phylogenetic tree constructed for Serpina10 orthologs and KLKB1 orthologs showed significant similarity. Docking pattern of the PK proteins from different organisms and the corresponding ZPI of those organisms also showed significant similarities. Conclusion: As the SerpinA10 gene known to exist before the divergence of cartilaginous fish, ZPI should have a significant function other than anticoagulation by interacting with the predecessor protease of FXI and Plasma pre-kallikrein.

PP-14

One-pot biogenic synthesis of gold nanoparticles@saponins niosomes: Sustainable nanomedicine for antibacterial, anti-inflammatory and anticancer therapeutics

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Abstract

Nanomedicine offers the promise of transforming modern medicine by facilitating precise and targeted therapeutic outcomes while reducing the adverse effects associated with conventional therapies. Nevertheless, the production process of nanomedicine often involves the use of hazardous and costly chemicals, leading to the creation of toxic by-products. This research paper presents a newly-developed, eco-friendly, one pot method of gold nanoparticles (AuNPs)@saponins niosomes synthesis by utilizing *Sapindus mukorossi* pericarps extract as both a reducing agent and stabilizer. The properties of the resulting AuNPs@saponins niosomes were analyzed in terms of composition, chemical structure, and morphology. Antibacterial activity of AuNPs@saponins niosomes was observed at concentrations of 50-100 µg/mL, and showed significant antibacterial effect on *Staphylococcus aureus*. The synthesized AuNPs@saponins niosomes also demonstrated potential as an anti-inflammatory agent, exhibiting an IC_{50} of 30.08 µg/mL, and displayed a dose-dependent anticancer effect against various human cancer cell lines up to 100 µg/mL. Among the tested cell lines, AuNPs@saponins niosomes exhibited the most effective cytotoxicity on MCF-7 cancer cells, displaying an IC_{50} of 54.13 µg/mL. Our results suggest that, this research has the potential to uncover the opportunities in the development of environmentally sustainable one-pot synthesis methods of metallic nanoparticles loaded niosomes, with applications in various fields for antibacterial, anti-inflammatory and anticancer therapeutics, offering promising avenues for advancement.

Keywords: Gold nanoparticles; Niosomes; Biogenic synthesis; Antibacterial Anticancer

PP-15

AI-Driven Material Discovery for Sustainable Polymers

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Abstract

The discovery of sustainable polymers is crucial for reducing environmental impact and promoting eco-friendly materials. Traditional methods of polymer research are time-consuming and costly, relying heavily on trial-and-error experiments. Artificial Intelligence (AI) offers a promising alternative by predicting polymer properties and performance before synthesis, speeding up the material discovery process. AI can process large datasets of polymer structures and properties to identify biodegradable, recyclable, and high-performance polymers, reducing the need for physical testing and leading to both cost and time savings. This study aims to develop an AI-driven model to discover sustainable polymers. Specifically, the model will predict biodegradability and recyclability, classify polymers based on environmentally friendly properties, and reduce the time and cost of polymer research through machine learning techniques. The process involves two primary steps: data collection and preprocessing using public datasets (e.g., PubChem, Kaggle) and machine learning model training with algorithms like Decision Trees, Random Forest, and Logistic Regression. Preliminary results demonstrate that the AI model can predict biodegradability with high accuracy, classifying materials based on desired properties and reducing the time and effort required to identify sustainable polymers. This approach can be extended to predict other properties, such as mechanical strength and thermal stability, and provides a foundation for future polymer research.

Keywords: Artificial Intelligence (AI), Sustainable Polymers, Machine Learning, Biodegradability, Recyclability, Polymer Research, Decision Trees, Random Forest, Logistic Regression

PP-16

Reactive Electrolyte Integration in $NiMnO_3$/ZIF-8 Nanocomposite for Enhanced Electrochemical performance for Supercapacitor Applications

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Abstract

Due to the increased energy requirements of the world, there is an increased demand for energy storage devices. Among the energy storage devices super capacitors are electrochemical energy storage devices that store and release energy by reversible adsorption and desorption of ions at the interface between electrode materials and electrolytes. The supercapacitance of the devices was based on the electrode materials used. Due to its high specific capacitance, good conductivity, ecologically friendly properties, inexpensive cost and abundance of material, $NiMnO_3$ is considered as a strong contender for super capacitor electrode materials. In this work $NiMnO_3$/ZIF-8 is synthesized using hydrothermal method. $NiMnO_3$/ZIF-8 has good stability and consequently, a possible material for high-rate super capacitors. ZIF based material integrated with $NiMnO_3$ to study the enhanced performance. The electrochemical behavior of the $NiMnO_3$/ZIF-8 electrode material was analyzed using three electrodes electrochemical workstation. The formation and morphological characteristics of the NiMnO3 materials were verified through systematic investigations. The structural and morphological studies were investigated through X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM). The electrochemical performance was executed by cyclic voltammetry (CV), galvanostatic charge and discharge (GCD) and electrochemical impedance spectroscopy (EIS).

Keywords: $NiMnO_3$, Composite, Electrochemical, Supercapacitor.

PP-17

Extraction of U(VI) from Aqueous Solution using Hydroxyapatite@g-C_3N_4 nanocomposite adsorbent

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Abstract

This study introduces a Hydroxyapatite@g-C_3N_4 nanocomposite (HAp@gCN) as an adsorbent for removing U(VI) ions from aqueous waste. Eggshell biowaste was used to produce hydroxyapatite through a simple precipitation method, whereas graphitic carbon nitride was synthesized via facile thermal condensation. FE-SEM, XRD, and FTIR were employed to assess the compositional and morphological features of HAp@gCN. Batch studies were conducted to examine U(VI) species sorption on HAp@gCN, considering factors such as pH, contact time, initial U(VI) concentration, adsorbent dosage, and ionic strength. FTIR, XRD, and EDS elemental mapping confirmed U(VI) adsorption onto HAp@gCN. The adsorption kinetics were aligned with a pseudo-second-order model and reached equilibrium within 90 min. The Langmuir isotherm model best described the adsorption isotherm data, with a maximum sorption capacity of 440.2 mg g^{-1} at 298 K. U(VI) can be extracted from the saturated adsorbent using 0.01 M HCl, and its sorption capacity remained stable even after four adsorption-desorption cycles. This research demonstrates that HAp@gCN nanocomposite has potential applications in environmental remediation as an eco-friendly material.

Keywords: Heavy metal ions, Adsorption, Hydroxyapatite, Carbon nitride, Nanocomposite

PP-18

Enhancing Performance and Stability of Carbon-based Perovskite Solar Cells with 1,2,4-Triazole Additive

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Abstract

Perovskite solar cells (PSCs) have gained immense interest due to their remarkable light-harvesting efficiency and high-power conversion efficiency (PCE). However, challenges such as defects and trap states within the perovskite layer continue to hinder optimal device performance by causing non-radiative recombination. This study introduces 1,2,4-triazole as an additive in the perovskite precursor solution to address these issues. The addition of 1,2,4-triazole significantly improved the quality of the perovskite film by reducing defect density, enhancing crystallinity, and passivating trap states. These improvements resulted in better charge carrier transport, minimized recombination losses, and enhanced device stability. CPSCs incorporating 1,2,4-triazole achieved a notable PCE of 10.66% and retained 85% of their performance after prolonged operation. These results highlight the potential of 1,2,4-triazole as an effective additive for improving the efficiency and long-term stability of perovskite solar cells.

Keywords: Perovskite solar cells, Carbon electrode, 1,2,4-Triazole.

PP-19

Doping Engineering of Ni with Co_3S_4 for Advanced Energy Storage Applications

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Abstract

Developing high-performance energy storage devices is crucial for next-generation sustainable energy systems. In this study, a Ni-doped Co_3S_4 nanocomposite is synthesized through a facile hydrothermal method and applied as an electrode material for solid-state asymmetric supercapacitors. Introducing Ni ions into the Co_3S_4 matrix enhances the electrochemical performance by optimizing charge transfer kinetics, increasing conductivity, and improving structural stability. Comprehensive characterization, including X-ray diffraction (XRD), Field emission scanning electron microscopy (FESEM), and energy-dispersive spectroscopy (EDS), confirms the successful incorporation of Ni within the Co_3S_4 lattice. The structural and morphological features of the nanocomposite are characterized using Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), and high-resolution transmission electron microscopy (HRTEM). The three-electrode system electrochemical measurements reveal superior capacitance, and excellent cyclic stability, compared to undoped Co_3S_4. When employed as the positive electrode in a Ni-doped Co_3S_4, paired with a reduced graphene oxide (rGO)-based negative electrode, the device exhibits a high energy density of 42.9 Wh/kg, impressive power density of 820 W/kg, and remarkable cycling stability with 90% retention after 10,000 cycles. These findings highlight the potential of doping engineering as an effective strategy for designing advanced electrode materials for high-performance energy storage systems.

Keywords: Ni-doped Co_3S_4; Transition metal sulfides (TMS); Doping engineering; Energy storage applications; Pseudocapacitive materials

PP-20

Sustainable and Efficient Anodizing for Automotive Plungers: Tackling Coating Defects and Improving Surface Finish

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Abstract

The anodizing process plays a crucial role in automotive plunger manufacturing by providing key benefits such as corrosion resistance, durability, and an aesthetically appealing surface finish. However, the process is often challenged by defects such as microfinish imperfections, smut formation, and powdery coating residues, which can significantly compromise the quality of the final product. These issues not only lead to increased rework and production costs but also raise concerns regarding customer satisfaction and operational efficiency. This review article examines the underlying causes of these common anodizing defects and explores the various strategies proposed in the literature to address them. It analyzes the influence of process parameters, chemical formulations, and environmental factors on surface quality and coating consistency. The review also discusses emerging techniques for optimizing anodizing processes to improve surface finishes, reduce energy consumption, and lower production costs, while maintaining compliance with stringent automotive quality standards. Emphasis is placed on developing more sustainable and efficient anodizing methods that enhance both the functional properties and aesthetic appeal of automotive plungers. By synthesizing current advancements, this article contributes to the ongoing efforts to improve process reliability and align the anodizing process with the automotive industry's environmental and economic goals.

PP-21

Synthesis, Characterization, and Antimicrobial Evaluation of Substituted Anthracene-Imidazole Derivative Integrated with Functionalized Chitin and Polyaniline on 3D-Printed Zirconia Oxide Composite

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Abstract

This study reports synthesizing and characterizing a novel composite material comprising substituted anthracene-imidazole derivatives, functionalized chitin, and polyaniline, integrated onto a 3D-printed zirconia oxide scaffold. The anthracene-imidazole derivative was synthesized through a multi-step condensation reaction between anthracene-based aldehydes and substituted imidazole precursors. Functionalization of chitin was performed to enhance biocompatibility and antimicrobial properties, while polyaniline was incorporated to provide electrical conductivity and mechanical reinforcement. Zirconia oxide was selected as the substrate due to its exceptional mechanical strength and biocompatibility, making it suitable for biomedical applications. The composite's structural and chemical properties were characterized using Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM), and thermogravimetric analysis (TGA). Antimicrobial activity was evaluated against various Gram-positive and Gram-negative bacterial strains, as well as fungi, using disc diffusion and minimum inhibitory concentration (MIC) assays. The composite exhibited significant antimicrobial efficacy, attributed to the synergistic effects of the anthracene-imidazole moiety and bioactive chitin derivatives. Polyaniline-enhanced 3D-printed zirconia oxide composites show potential for advanced biomedical applications like antimicrobial surfaces, implants, and tissue engineering scaffolds. This novel material design offers potential strategies for combating microbial resistance while providing structural and functional versatility for dental devices.

PP-22

Biocompatible HNT/Mg/Zn-HA-PLA Coatings for Titanium Implants in Osteosarcoma Treatment and Bone Defect Repair

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Abstract

Tooth and bone loss is a global concern, driving research into biomaterials for dental implants. Effective osteosarcoma treatment focuses on eradicating the disease, restoring bone defects, and preventing infections. Titanium, a commonly used metallic material, offers exceptional biocompatibility, high stiffness, and excellent corrosion resistance. Among these materials, synthetic hydroxyapatite (HA) stands out as a fully biocompatible and osteoconductive material that closely resembles the structural and chemical composition of natural bone mineral. This unique property enables HA to interact with living bone tissue, mimicking the behavior of natural bone. Furthermore, biomaterials like HA exhibit osteoprotective and osteostimulatory properties, which, when exposed to tissue fluids, promote the proliferation and differentiation of osteoblast cells. In this study, we developed a titanium implant substrate coated with HNT/magnesium/zinc-doped hydroxyapatite (HNT/Mg/Zn-HA) powder using a wet precipitation method. This was then combined with polylactic acid (PLA) as an ink to form a composite, which was ultimately applied in the repair of bone defects caused by malignant osteosarcoma. This process facilitates the formation of an extracellular matrix and supports mineralization, thereby enhancing bone regeneration. An in vitro cell viability assay was conducted using MG-63 osteoblast cells on the optimized coating obtained at 4000 RPM, demonstrating excellent biocompatibility with the cell line. Additionally, corrosion resistance was evaluated through polarization and EIS studies, which revealed outstanding corrosion resistance properties of the coating. In summary, the (HNT/Mg/Zn-HA) PLA composite developed in this study proved effective in tumor treatment, bone defect repair, and post-operative infection prevention. It holds significant potential as a simple yet powerful therapeutic material for osteosarcoma resection, enhancing bone cancer elimination.

PP-23

Enhanced Surface of 316L Stainless steel with incorporating Mineral-HAP/ Sulfate polysaccharide and Advanced Polymer: Biomedical Applications

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Abstract

Advanced biomedical implants require materials with high biocompatibility, bioactivity, and mechanical qualities. The current research aims to improve the surface of 316L stainless steel by integrating mineral-based hydroxyapatite and functional additives, which are a type of biocompatible and renowned for their favorable effects on cellular activity. The surface coating also included sulfate polysaccharides originating from natural sources and a family of synthetic polymers known for their mechanical stability. These materials were produced using wet precipitation and then applied to the 316L SS substrate using electrospinning methods. Hydroxyapatite (HAp) stands out as a non-toxic, bioactive ceramic increasingly employed as a biocompatible coating material. It offers superior osteoconductivity, and the functional modifications improve mechanical stability and bioactivity. While the incorporation of rare earth minerals into HAp is expected to enhance the surface strength of the coating. The synthetic materials contribute in controlled degradation and mechanical reinforcement, Sulfate polysaccharides are well known for being utilized in drug delivery (DD), and tissue regeneration (TE), enhancing biocompatibility and encouraging attachment between cells. The successful integration of these materials was confirmed by thorough physiochemical investigations using XRD, FT-IR, SEM with EDAX, and TEM. Cell viability and Proliferation tests, among other Biological assessments, showed enhanced bioactivity and cytocompatibility. An important advancement in the creation of multifunctional biomedical implant materials was made when the optimized composite coating showed promise for use in dental and orthopaedic implants.

PP-24

Biopolymer Chitosan based smart Photodynamic Drug Delivery - a futuristic view

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Abstract

Chitosan is a cationic polysaccharide which lends itself to functionalization to give different derivatives owing to involvement of amino, acetamido and hydroxyl moieties in the ring.[1] Chitosan based polymeric biomaterials are extensively used in biomedical applications due to their outstanding biocompatibility and biodegradability. We can design multi-functional chitosan biomaterials with various functional groups for specific biomedical applications.[2-3] They are widely used in regenerative medicines,[3] drug delivery[1,3] and tissue engineering.[4] Therefore, this talk will briefly introduce the concepts and progress of photo-sensitizer coated chitosan biomaterials, the need for these technologies in the fields of drug delivery and tissue engineering, and their potential applications. Furthermore, future opportunities to develop, challenges, and strategies for chitosan based polymeric biomaterials in smart photodynamic drug delivery and tissue engineering are offered as added advantages.

Keywords: *Chitosan; Functionalization; Photodynamic drug delivery; Regenerative medicines; Tissue engineering*

PP-25

Synergistic Activity of $SrFeO_3/TiO_2$ Nanocomposites for Biodiesel Production

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Abstract

$LaFeO_3$, TiO_2 nanoparticles (NPs), and $LaFeO_3/TiO_2$ nanocomposites were synthesized and evaluated for their potential in biodiesel production through photocatalytic transesterification reactions under UV light. XRD analysis confirmed the orthorhombic and rutile phases of $LaFeO_3$ and TiO_2, respectively, with the composite retaining the distinct phases of both materials. Morphological studies revealed spherical nanoparticles with an average particle size of approximately 60 nm for $LaFeO_3$, TiO_2, and $LaFeO_3/TiO_2$. The UV-Vis absorption spectra of the $LaFeO_3/TiO_2$ nanocomposites showed enhanced light absorption compared to individual TiO_2 and $LaFeO_3$ nanoparticles, facilitating higher photocatalytic activity. Under optimized conditions, including a 4:1 alcohol-to-oil molar ratio, 100 mg of $LaFeO_3/TiO_2$ catalyst, a 100-minute reaction time, and 80 °C temperature, the composite achieved a biodiesel yield of up to 81%. This performance is attributed to the synergistic properties of the composite, enhancing its photocatalytic efficiency. Furthermore, the $LaFeO_3/TiO_2$ nanocomposite exhibited excellent stability and reusability, maintaining consistent catalytic efficiency over five cycles. These findings highlight the potential of $LaFeO_3/TiO_2$ nanocomposites as effective and sustainable photocatalysts for biodiesel synthesis.

Keywords: $LaFeO_3@TiO_2$ NC; Catalytic Activity; Reusability; Biodiesel;

PP-26

An Enzymeless Biosensor Based on Ni-CuO nanoparticles

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Abstract:

The detection of Glucose is of interest especially the past decades due to the increasing number of persons with diabetes and other disease conditions effecting the human body. The continuous monitoring of glucose provides for early and effective treatment options. Though various techniques are available for glucose detection, there still arises the need for cost effective, stable, sensitive, selective and reproducible sensors. Herein we have used green synthesized Ni-CuO nanoparticles as electrocatalyst for the non-enzymatic detection of glucose. The Ni-CuO nanoparticles were synthesized via by a simple precipitation method and used to fabricate an electrochemical sensor for glucose detection. Techniques like Fourier transform infrared spectroscopy (FT-IR), Scanning electron microscope (SEM), UV-Vis spectroscopy and voltammetry has been utilized to thoroughly characterize the surface of the sensor and study the electrochemical detection. Differential pulse voltammery was used to determine various concentration of glucose and showed a detection limit of 3.26 nM with a linear range between 9.8 and 33.09 nM. The Ni-CuO based electrochemical sensor showed good stability, reproducibility and quick response. Further amperometric detection showed interference free response for glucose.

PP-27

Electrochemical Detection of Nitrite Using Graphene Oxide Silver Nanosuspension

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Abstract

Nitrite is added as preservative which upon reaction with amines and amides can result in the formation of nitrosamines, many of which are carcinogenic. Hence, from a health point of view the detection of nitrite becomes very important. Herein we have devised an electrochemical sensor using Graphene Oxide - Silver nanosuspension (GO-Ag NS) for the detection of Nitrite. Graphene Oxide (GO) was prepared using Hummer's method and Silver nanosuspension (Ag NS) was prepared via a sunlight mediated reduction process using *Cathranthus roseus* leaf extract as a reducing agent. The GO-Ag NS suspension was dropcasted on a graphite electrode and thoroughly characterized using UV-visible spectroscopy, Infrared Spectroscopy, and Scanning Electron Microscopy. For the electrochemical sensing of nitrite, voltammetric technique was used in 0.1 M Phosphate buffer of pH 6 after optimizing the condition for best detection. The linear Range for detection of nitrite using the modified electrode was found to be 1 nM to 15 nM with a limit of detection of 0.33 nM. Repeatability, reproducibility and stability studies shows satisfactory results. The sensor was also subjected to real sample analysis and the recovery percentages obtained vary between 98 to 99.4 %. The sensor thus showed promise for application in food safety field and also in environmental field.

Keywords: Nitrite; Electrochemical Detection; Voltammetry; Silver Nanosuspension; C. Roses

PP-28

A novel curcumin-loaded PLGA micromagnetic composite system for controlled and pH-responsive drug delivery

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Abstract

Poly (D, L-lactide-co-glycolic acid) (PLGA) based magnetic microspheres (MMS) hold immense potential for reaching the target of controlled and specific drug delivery site with low toxicity. Herein, we have synthesized the biodegradable PLGA microspheres (MS) containing magnetic iron oxide nanoparticles (MIONPs) by the emulsion solvent evaporation method and loaded (them) with the well-known anti-cancer drug, curcumin. The existing crystallinity of MIONPs in the MMS has been confirmed by powder XRD analysis. The prepared MMS displayed excellent superparamagnetism displaying a saturated magnetism with a value being 24.4 emu/g. The morphology of MS and MMS was found to have spherical shape along with a smooth surface of mean diameter of 0.5 μm and 1 μm (micrometer range). Moreover, the MIONPs content of 23.74 wt% in the MMS was evaluated referring TGA studies. However, the drug release profiles resulted that the MMS have a pH-induced drug-releasing asset with a cumulative CUR releasing efficiency of 73.25%. According to the results obtained from the cytotoxic studies, MMS has cytotoxicity against HeLa cell lines with a significant potency that is promising for targeted chemotherapeutic applications.

Keywords: Drug delivery; PLGA microsphere; Curcumin; Controlled drug release; pH-responsive

PP-29

Reinforcement Learning-Based Predictive Thermal Management for GaN Power Inverters under Variable Driving Cycles

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Abstract

The growing use of electric vehicles (EVs), and the need for advanced thermal management technologies, especially GaN-based power inverters, has increased. These inverters are high in density and efficiency but can overheat resulting in static thermal management integration being inefficient in maintaining the conditions. To overcome the challenge, the study had a solution that utilized dynamic thermal management. This consists of real-time monitoring and predictive models, reinforcement learning methods, and automated cooling control systems. By the use of reinforcement learning, the system has been able to optimize various cooling protocols in real time during different operating conditions. The RL agent employing a Q-learning algorithm, learns to adjust cooling system parameters dynamically—such as fan speed and coolant flow rate-while balancing efficiency and safety. A strategic reward system optimises inverter temperature control across driving modes using heat sinks and PCMs to ensure safe temperatures and energy-efficient cooling. Through the use of MATLAB simulation and subsequent experiments, it had been indicated that the system was able to beat statically controlled systems. Thereby, reducing the peak ceiling temperatures by 15-20 percent and increasing cooling efficiency by 25 percent. This approach subsequently managed to remove thermal bottlenecks and enhance the system's performance and dependability. Future research will emphasize a more sophisticated thermal management strategy through an even more intelligent combination of smart sensors and AI augmentation techniques in smart-enabled hybrid cooling systems.

PP-30

Reinforcement Learning-Driven Optimization of GaN-Based Power Amplifiers for 5G: Achieving Enhanced Linearity and Reduced Intermodulation Distortion

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Abstract:

Gallium Nitride (GaN) is a Wideband semiconductor which play a crucial role in the development of high-performance power amplifiers (PAs) for 5G communication systems. GaN's high electron mobility, breakdown voltage, and thermal stability address 5G requirements of high data rates and reliability. However, optimizing GaN-based PAs for 5G presents significant challenges, particularly in enhancing linearity and reducing Intermodulation Distortion (IMD) during wideband signal transmission. These nonlinearities and distortions can reduce signal quality, cause interference with adjacent channels, and have an impact on overall system performance. In order to overcome these challenges, this study employes dataset-driven approach to optimize the performance of PA by combining reinforcement learning (RL) with Proximity Policy Optimization (PPO). A custom reward function had maintained acceptable trade-offs between different metrics like IMD3, Gain, efficiency, output power, input power. The system had been achieved the most efficient optimization accuracy of 98.18% with an IMD3 penalty weight of 10 and reward weight of 5, effectively reducing IMD3 while enhancing gain and efficiency in GaN-based power PAs for 5G networks. This ensures superior signal quality, reduced interference, and reliable performance in dense 5G environments. The results facilitate efficient 5G device design, with future work to focusing on mm Wave and beyond-5G challenges.

PP-31

Structural Analysis of 4-Bromomandelic Acid as a Potent M2 Muscarinic Receptor Antagonist: A Molecular Docking Study

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Abstract:

The M2 subtype of the muscarinic acetylcholine receptor (mAChR) plays a vital role in regulating cardiac, respiratory, and central nervous system functions. Homatropine, a recognized anticholinergic agent, antagonizes mAChRs, providing therapeutic benefits such as pupil dilation, reduction of uveal tract inflammation, and suppression of cough reflexes. This study employs molecular docking techniques to investigate the interactions of 4-bromomandelic acid, a novel derivative of homatropine, with the human M2 muscarinic receptor (PDB: 3UON). Structural modifications of homatropine were designed to enhance its binding affinity and receptor specificity. The ligand preparation involved molecular modeling, including energy minimization and topology generation, followed by docking simulations to predict its binding conformations and interaction profiles within the M2 receptor's orthosteric site. Key interactions such as hydrogen bonding, hydrophobic contacts, and halogen bonding were examined to assess their contributions to receptor binding. Docking outcomes indicated that 4-bromomandelic acid exhibited significantly enhanced binding affinity compared to the parent homatropine molecule. The bromine atom was found to promote halogen bonding and strengthen hydrophobic interactions, leading to the observed improvement in affinity. Insights into the structure-activity relationship (SAR) were obtained by analyzing the key amino acid residues involved in binding. This study highlights 4-bromomandelic acid as a promising M2 receptor antagonist with improved binding properties. The findings contribute to the understanding of SAR in homatropine derivatives, laying the groundwork for the development of more potent and selective anticholinergic agents. Future research will focus on in silico ADMET profiling and molecular dynamics simulations to assess the pharmacokinetic and pharmacodynamic properties of this derivative.

PP-32

Mineral analysis of soil samples affected by tanning activities

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Abstract:

Tanning activities can significantly alter the mineralogical composition of soil, which influences the soil functions and environmental quality. This present study aims to identify the mineral composition in the soil samples affected by the tanning activities in the leather industrial areas of Tamil Nadu. Using Fourier transform infrared (FT-IR) spectroscopy and X-ray diffraction (XRD) techniques, the mineral analysis was performed. From the results of FT-IR and XRD, the presence of clay minerals, such as halloysite, montmorillonite, kaolinite, and chlorite; iron oxides, such as hematite and goethite; carbonate mineral, such as calcite; magnetic minerals, such as magnetite, hematite, and ilmenite; as well as the resistant minerals such as quartz, zircon, and rutile. Some of the minerals, such as halloysite, montmorillonite, chlorite, biotite, magnetite, hematite, goethite, ilmenite, and apatite, minerals can adsorb or react with heavy metals, particularly chromium, in certain oxidizing or reducing conditions. This interpretation clearly indicates that the soil could be affected by the tanning activities in the study area.

Keywords: Mineralogy; Soil; FT-IR; XRD; Tanning

PP-33

Magnetic susceptibility measurements in leather industrial soil samples

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Abstract:

Magnetic susceptibility of soil samples collected from leather industrial areas of Tamil Nadu was explored using Bartington MS2B dual frequency susceptibility meter at both low and high frequencies. All the samples show that magnetic susceptibility at low frequency is slightly higher than the magnetic susceptibility values at high frequency. And also, the magnetic property and the presence of super paramagnetic (SP) grain sizes in the soil samples were identified by calculating percentage of frequency dependent susceptibility (χfd%). All samples have the magnetic susceptibility value χ>100. From the results of χfd%, some samples have no contribution of SP grains and others have mixture of SP and coarser non-SP grains. These magnetic variations in the soil samples are occurred due to the anthropogenic activities in the study area.

Keywords: Magnetic susceptibility; Soil samples; Leather industry; Tamil Nadu

PP-34

Enhancing Corrosion Resistance of Iron with Copper Nanoparticles and Polymer Coatings

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Abstract:

The purpose of this study is to address the significant issue of corrosion of iron in machinery. Temporary solutions such as paint, oil, and grease provide short-term protection, while long-term durability is achieved by coating iron with corrosion-resistant materials. This research investigates the effectiveness of coating iron strips with copper nanoparticles using the electrodeposition method. To prevent oxidation of the copper nanoparticles, the strips were further coated with polyvinylidene fluoride (PVDF) via dip coating. The stability of the coatings was evaluated through mechanical testing, atmospheric exposure, and characterization techniques, including scanning electron microscopy (SEM). Results demonstrate that the iron strips coated with copper and PVDF exhibit reduced corrosion rates compared to uncoated samples. These findings suggest that PVDF/copper coatings provide a promising approach to enhancing the lifespan of iron components in various industrial applications.

PP-35

Synthesis Of Organometallic Ruthenium(Ii) Complexes Containing Carboxamide Ligands Appended Heterocyclic Rings

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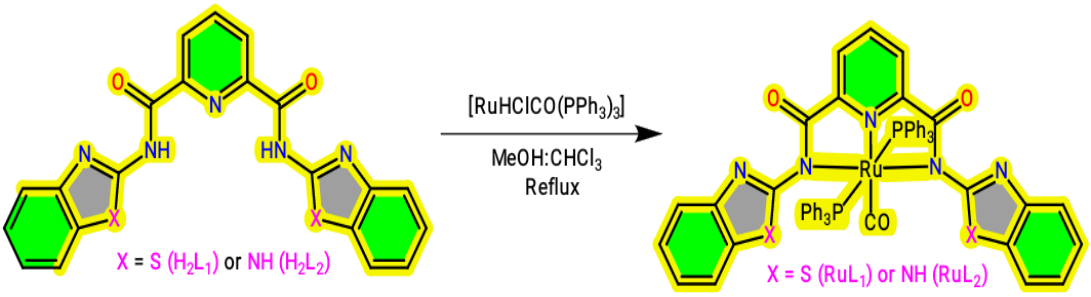
Abstract

Synthesis of new ruthenium(II) complexes appended ligand N_2,N_6-di(benzo[d]thiazol-2-yl)pyridine-2,6-dicarboxamide/N_2,N_6-di(1H-benzo[d]imidazol-2-yl)pyridine-2,6-dicarboxamide and their ruthenium(II) were synthesized. The characterization of the ligand and its complexes were accomplished by analytical and spectral (UV-Vis, IR, NMR and ESI-MS) methods. In these complexes, the Ru(II) ion was exhibited a distorted octahedral geometry with a tridentate NNN donor fashion while the remaining coordination sites were occupied by either anionic neutral co-ligands such as CO and PPh_3.



Keywords: Ruthenium (II) complexes, Pyridine-carboxamide ligand, Octahedral geometry

PP-36

Redefining The Nanomaterial Nanoarchitectonics for The Development of Self-Assembled Biomass Derived Carbon Architecture

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Abstract

The use of biomass derived carbon is limited and to exploit its fullest potential. In this work, the authors would like to propose a strategic development of self-assembled carbon nanoarchitecture with help of Nanoarchitectonics concept. The Nanoarchitectonics is a concept involving classical supramolecular chemistry, materials science and biological science for the development of advanced functional nanomaterials. The self-assembled superstructures are reported and holds a great interest in the material and synthesis science for fabrication and discovery of novel materials with distinct characteristic properties. Previously, reported nanostructures like fullerenes and fullerene-based assemblies, carbon nanotubes (CNTs), graphene and graphene based materials and carbon quantum dots (CQDs) are some of the nanomaterials which had impacted the science and technology for varied applications. This constructive conceptualisation of biomass derived nanoassembly will redefine the nanomaterial science and engineering with potential in energy storage to biomedical applications. The exploitation of biomass derived superstructures with defined morphology will be the material of future. The exploration of a new material space begins here!

PP-37

Fabrication of Sustainable Cellulose Nanocrystal-Based Hydrogel Beads Incorporating Green-Synthesized Magnetic Nanoparticles for Efficient Adsorption of Aquatic Pollutants

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Abstract

Environmental pollution from contaminants poses significant risks to ecosystems and human health. The growing presence of emerging contaminants (ECs) in water has become a global challenge, aligning with the priorities of the UN 2030 Agenda for Sustainable Development Goals. Hydrogels, with their three-dimensional porous structure and low density, offer considerable potential for tackling this issue. In particular, cellulose nanocrystal (CNC)-based hydrogels, derived from renewable and biodegradable resources, are promising for adsorption applications. However, their inherent hydrophilicity limits their effectiveness in water and wastewater treatment. To address these challenges, incorporating advanced components and applying targeted modifications are crucial. Magnetic nanoparticles (MNPs) have emerged as valuable additions due to their high surface area, magnetic properties, and functional versatility. This work explores the synthesis, modification, and application of CNC-MNP hydrogel beads to enhance adsorption efficiency for diverse environmental contaminants. By addressing hydrophilicity challenges and creating stable composite systems, CNC-MNP hydrogel beads present a sustainable and efficient approach for promoting cleaner ecosystems and safeguarding public health.

PP-38

Green Synthesis of Iron Oxide and Calcium Oxide Nanoparticles from Orange Peel and Oyster Shell Waste for Wastewater Treatment

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Abstract

Industrial growth has led to a significant rise in water pollution, with dyes being major contributors to contamination. Effective removal of dyes from wastewater has garnered considerable attention, with adsorption using nanosorbents emerging as a promising solution. In this study, calcium oxide (CaO) and iron oxide (Fe_2O_3) nanoparticles, synthesized via an environmentally friendly green synthesis method, are employed as adsorbents for dye removal. Green synthesis utilizes natural precursors such as orange peel waste, rich in antioxidants and vitamin C, and oyster shells, known for their biosorption properties. The nanoparticles were characterized using UV-Vis spectroscopy, revealing particle size ranges of 230–330 nm for CaO and 230–290 nm for Fe_2O_3 nanoparticles. Adsorption process parameters, including temperature, pH, contact time, and adsorbent dosage, were optimized to maximize dye removal efficiency. Structural and morphological properties were analyzed using SEM, XRD, FT-IR, and TEM techniques. Additionally, adsorption behavior was evaluated using isotherm and kinetic models. This study highlights the potential of green-synthesized CaO and Fe_2O_3 nanoparticles as sustainable and efficient nanosorbents for water treatment applications.

Keywords: *calcium oxide, iron oxide, nanoparticles, dye removal*

PP-39

Studies on Customization and Scalability in Scaffold Design Using 2D Material for Tissue Regeneration

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Abstract

Tissue regeneration is a process of replace the damage tissue for particular parts of body, tissue or organ. The 2D materials are used in various application like photovoltaics, semiconductors, electrodes, water purification, drug delivery, bio sensing and tissue regeneration. Two dimensional materials are crystalline solids consisting of a single layer atom. The 2D materials can be produced mainly by two approaches top down exfoliation and bottom up synthesis. The 2D material has a great potential in biological application due to various chemical and physical surface properties. The 2D material combines with biomaterial to increase biocompatibility and host response property. Two dimensional materials like graphene oxide, black phosphorus, MXenes are used in tissue regeneration. These materials are used to replace and repair tissue in bone, cartilage and nerve. Graphene is the widely used 2D carbon material to produce scaffolds for various tissue like bone, cartilage and brain. This material is act same as extracellular matrix which helps cells to adhere, differentiate and proliferate. The advantages of graphene in tissue regeneration as mechanical strength, electrical conductivity and cell adhesion. The fabrication of scaffolds by 2D material has done by various techniques like electrospinning, 3D printing, sol gel method. The controlled addition of 2D material to the scaffold matrix to achieve desired function of the selected tissue. As per the future aspect we also consider the scalability, toxicity and regulatory approvals for sustainable development in tissue engineering.

PP-40

2D Nanomaterials for Target Drug Delivery of Lymphoma

Mahalakshmi Balakrishnan[a], Jason Thamizhakaran Stanley[b], Shanmuga Sundar Saravanabhavan[a], Amudha Thanarasu[c], Sathya Selva Bala Vasanthakumar[d], Jacklien Emema Rose T.J. [b], Jeny Rachel Biju[b], Baskaralingam Palanichamy[e], Anuradha Dhanasekaran[f], Sivanesan Subramanian[b*]*

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Abstract

Drug delivery is a process to deliver a drug in human or animal to achieve its medicinal effect. The efficiency of the drug delivery is a measure, how well drug is delivered to a planned target. There are many diseases that can be used to treat in drug delivery with the help of 2D materials. The lymph glands are unique part of a human body which acts the body's disease-fighting network. It mainly includes the lymph nodes, present in underarms, armpits and groin. The lymphoma cancer, is a prominent cancer affecting the lymphatic system. The major treatment involved in chemotherapy, medication, radiation therapy, and stem cell transparent. 2D Materials are nanomaterials which is have ultrathin layered materials combined with a high surface to volume ratio that can deliver many therapeutics including small molecule drugs, peptides and large proteins. Their high surface area allows for high therapeutic loading and prolonged therapeutic release over time (examples of 2D materials using for lymphoma cancer: graphene, molybdenum disulfide MoS_2) 2D materials can be used as diagnosis and treatment of lymphoma cancer. They can be used as biosensor to detect lymphoma and as a drug carrier for targeted drug delivery. As per the future aspects of 2D materials in lymphoma cancer targeted drug delivery, personalized medicine, combination therapy, immunotherapy.

Keywords: *Targeted drug delivery, Drug carriers, 2D Nanomaterials, Lymphoma*

PP-41

Grading of serum albumin using dynamic light scattering setup

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Abstract

Dynamic light scattering (DLS) is a non-invasive method that can quantify particles' dimensions in the eye's aqueous humor during inflammation due to uveitis. The bovine serum albumin (BSA) was chosen as a biomarker for anterior uveitis, and its particle size is measured using the Litesizer 500 DLS instrument and custom-built lock-in amplifier (LIA) based DLS setup. Using Litesizer 500, the hydrodynamic diameter, polydispersity index, and diffusion coefficient varied with concentration, with a positive correlation between concentration and hydrodynamic diameter. The intensity-weighted particle size distribution showed heterogeneity due to aggregates of BSA in distilled water. The hydrodynamic diameter remained identical for all the samples when measured using an LIA-based DLS setup. DLS can be a simple tool to quantify the proteins and cells during uveitis conditions. Nevertheless, the LIA-based custom-built DLS setup must be enhanced using focusing lenses to efficiently detect the light scatter emitted by the diffused particles.

Keywords: Dynamic light scattering, uveitis grading, aqueous humor, protein, lock-in amplifier

PP-42

Machine Learning Framework for Predicting Drug Delivery Outcomes Using Patient Response Data: A Focus on Breast Cancer Treatment

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Abstract

The increasing complexity of drug delivery systems in breast cancer therapy necessitates advanced machine learning (ML) techniques for precise prediction and optimization. Previous studies have utilized various ML approaches, but often face challenges related to interpretability, scalability, and real-time performance. This study addresses these gaps by integrating Random Forest and XGBoost models to predict drug delivery outcomes using patient response data from six breast cancer cases. Significant features such as "Avg_AUC" and "Threshold" were employed to develop predictive models. Both models demonstrated high performance, achieving close accuracy, precision, recall, and F1 scores. However, XGBoost outperformed Random Forest, providing higher confidence in predictions and lower logarithmic loss. The study's methodology includes preprocessing the data, selecting significant features, segmenting the data into training and testing sets, and evaluating the models against standard metrics. This approach effectively bridges the gap between traditional ML methods and the need for real-time, scalable solutions. The results highlight the efficacy of XGBoost in achieving superior predictive accuracy and confidence in drug delivery outcomes. Future research will focus on refining these models by incorporating cutting-edge materials science approaches, optimizing their performance through innovative computational techniques, and further enhancing their application in clinical settings. Additionally, future studies will explore the integration of cloud-based solutions and edge computing to improve data scalability, real-time processing, and collaborative capabilities in handling complex material-based data.

Keywords: Targeted Drug Delivery, Breast Cancer Treatment, Machine Learning, Data Preprocessing, Drug Delivery.

PP-43

Synthesis of Mn-Doped Bi_2O_3 nanoparticles for detection of allura red using electrochemical sensor

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Abstract

The innovative development and application of a nanosensor to identify dangerous Allura red food dye are presented in this work. Manganese-doped Bismuth nanoparticles (Mn-Bi_2O_3) were drop cast on graphite electrode (GE) surface to develop this sensitive platform. Mn-Bi_2O_3 -GE was used to demonstrate the sensing capabilities of the proposed nanosensor using electrochemical measurement, differential pulse voltammetry, and Cyclic voltammetry. The optimal response conditions for the target analyte were optimized through the examination of multiple parameters. In contrast to the unmodified GE, the investigation showed that the Mn-Bi_2O_3 GE greatly increased the signals of the Allura red food dye. The linear range of Allura red is 1µM to 5µM. The highest reaction was observed at pH = 8. The electrochemical sensing probe showed a strong linear correlation between Allura red concentration and current, with limits of detection (LOD) and quantification (LOQ) of 0.5018µM and 1.139µM, respectively. The correlation coefficient R^2 is 0.99. The sensitivity of the developed sensor is 12.5840 µA μM^{-1} cm^{-2} . Under optimal circumstances, the Bi-MnO_2-GE system can detect Allura red with a low limit of detection and has high sensitivity. Furthermore, the proposed electrochemical platform's remarkable stability, sensitivity, and repeatability point to its possible use in actual sample analysis.

PP-44

Microwave assisted synthesis, spectral characterization of dimethylthiazolidine-4-ones for medicinal application: Docking Investigation

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Abstract

A series of novel dimethylthiazolidine-4-ones (**1 - 4**) were synthesized using recyclable and environmentally benevolent Amberlite IR-120H resin as a unique and highly efficient catalyst with microwave irradiation. All the synthesized compounds were characterized by FT-IR, ^{1}H and ^{13}C NMR spectral studies. In all the compounds, the observed vicinal coupling constants and chemical shifts suggest that**,** piperidin ring adopts chair conformation with equatorial orientations of the aryl groups and the methyl group at C-3 should be equatorial. Two isomers such as ***E*** and ***Z*** were formed in all the compounds. Antibacterial, antifungal and antimycobacterial studies were carried out. The minimum inhibitory concentration values of the compounds in both antibacterial and antifungal activities suggest that all the compounds shown good activity against all the tested bacterial and fungalstrains. Dimethylthiazolidin-4-one(**1)** is more active against *Staphylococcus aureus* compared to the standard drug *Streptomycin*. Meanwhile, in antifungal studies, the compound **1** is more active against *Candida albicans* and *Aspergillus flavus* compared to the standard drug *Amphotericin B*. Also, it displayed good anti-tubercular activity against mycobacterium tuberculosis $H_{37}Rv$.These antibacterial, antifungal and anti-tubercular activities are mainly due to the presence of the electron withdrawing group in the aryl moiety. The docking investigation results the scores for compounds 1-4 were recorded as follows: -4.856, -3.788, -4.464, and -5.406 kcal.mol^{-1}.

PP-45

Optimization and characterization of sophorolipid functionalized silver nanoparticles (SL-AgNP) by *S. bombicola*.

Heeranshi Jain, Vasundhra S, Aarchisha Jha, Dr. V Vinoth Kumar, Priyadharshini Bharathi

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Abstract

Overusing chemical pesticides and surfactants adversely affects plants. Sophorolipid-stabilized silver nanoparticles (SL-AgNPs) provide a sustainable, eco-friendly alternative to combat fungal and bacterial infections while reducing chemical dependence. This innovative approach addresses key agricultural challenges, enhancing crop protection and productivity. In this study, the production of sophorolipids was optimized using the yeast Starmerella bombicola and evaluated their potential applications in agriculture as fungicides and bacteriocides. The highest yield of SL was observed on day 3, as determined by characterization. To enhance the functional properties, SL-AgNPs were synthesized using AgNO3 solution. In the production of AgNPs, sophorolipid acted as capping and reducing agents. To create uniformly sized and stable nanoparticles, crucial parameters such as pH levels, reaction times, and sophorolipid and silver nitrate concentrations were optimized UV-Vis spectroscopy confirmed the formation of nanoparticles with a peak observed at 420 nm. Dynamic light scattering (DLS) analysis revealed an average particle size of 85 nm, while zeta potential indicated a surface charge of 21 mV, confirming the stability and uniformity of the nanoparticles. Antimicrobial activity tests demonstrated inhibitory effects of SL-AgNPs against *E coli* and *Staphylococcus aureus*, the zones of inhibition measured 2 cm in diameter, whereas for antifungal activity it showed 1.5 cm for *Phoma* and *Fusarium typhinulum*. Comparatively, crude sophorolipids exhibited a lower inhibition zone of 1.2 cm, highlighting the enhanced bioactivity of SL-AgNPs. Further it was confirmed by characterization including Fourier Transform Infrared (FTIR), MBC and MFC. The study establishes the potential of these nanoparticles in agriculture as efficient sustainable fungicides and bactericides. Their ability to inhibit the growth of pathogens highlights their applicability in controlling infections, reducing reliance on chemical pesticides. Future studies will focus on large-scale production, field trials, and formulation optimization.

DAY 2 - 04.02.2025

POSTER SESSION - II

(10.45 AM to 11.35 AM)

Venue: Central Seminar Hall

(ECE Annexure)

PP-46

Various Characterisation Techniques Involved in Material Synthesis and Synergistic Development of Analytical Approach

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Abstract

Characterisation procedures are methods for analysing the physical, chemical, and structural properties of materials both during and after synthesis. XRD, SEM, FTIR, and NMR are essential for confirming synthetic processes and assuring material quality. These methods are commonly used in industries such as electronics, medicines, and nanotechnology. XRD determines crystalline phases, SEM studies surface characteristics, FTIR detects functional groups, and NMR investigates molecular interactions. X-ray photoluminescence spectroscopy and high resolution transmission electron microscopy also plays an important role in understanding the materials characteristic nature. With this reliable techniques creation and development of innovative materials including catalysts, polymers, composites, and energy storage devices is feasible. Future developments could include incorporating AI/ML for faster data interpretation, hybridising approaches (for example, mixing XRD and Raman spectroscopy), and miniaturising equipment for portability and cost efficiency. The development of ultrafast, high precision and non-destructive characterisation techniques would be displaying its proficiency in sophisticated equipment utilisation for material analysis with cost effective method. Characterisation processes are critical for material innovation. Future research should focus on improving accuracy, accessibility, and efficiency in order to fulfil expanding technological needs with advanced analytical techniques.

PP-47

The 2D Nanoarchitectonics on Development of Flexible Supercapacitor Device

Udayashamini Udayakumar[a], Jason Thamizhakaran Stanley[b], Amudha Thanarasu[a], Shanmuga Sundar Saravanabhavan[c], Sathya Selva Bala Vasanthakumar[d], Jacklien Emema Rose T.J. [b], Jeny Rachel Biju[b], Baskaralingam Palanichamy[e], Sivanesan Subramanian[b*]*

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Abstract

Supercapacitors are advanced energy storage devices known for their ability to charge quickly, have long lifespans, and deliver rapid bursts of energy. Supercapacitors are categorized into three types: Electrochemical Double-Layer Capacitors (EDLCs), which store energy through charge separation for long-lasting performance; Pseudocapacitors, which utilize redox reactions to provide higher energy density; and Hybrid Supercapacitors, which combine both types to optimize energy and power density. The integration of 2D materials such as graphene, MXenes, Transition Metal Dichalcogenides (TMDs), and Black Phosphorus enhances the efficiency of supercapacitors by offering high surface area, superior conductivity, and flexibility. Nanoarchitectonics is a modern approach that merges nanotechnology with other fields like supramolecular chemistry, self-assembly, self-organisation material science for controlling material sizes. Flexible supercapacitors, which can bend and stretch without losing effectiveness, are particularly valuable due to high capacity, longer cyclability, low cost and ease of fabrication. The 2D nanarchitectonics enables the development of flexible supercapacitor with tailored and enchanced energy density, conductivity, and mechanical adaptability, making them ideal for advanced applications like wearable electronics, smart textiles which can plays a key role in developing these flexible supercapcitor devices in applications requiring lightweight, durable, and portable energy storage, such as wearable electronics, smart fabrics, and flexible displays for portable and wearable electronics.

PP-48

The Transition of 2D Nanomaterials for Energy Storage Devices

Subash Selvakumar[a], Jason Thamizhakaran Stanley[b], Amudha Thanarasu[a], Shanmuga Sundar Saravanabhavan[c], Sathya Selva Bala Vasanthakumar[d], Jacklien Emema Rose T.J. [b], Jeny Rachel Biju[b], Baskaralingam Palanichamy[e], Sivanesan Subramanian[b*]*

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Abstract

Energy storage is essential for a stable, sustainable, and efficient energy future as it increases industrial efficiency, lowers costs, ensures energy security, and stabilizes the power grid by managing peak loads. As the demand for high-performance energy storage grows, advanced materials like 2D nanomaterials become increasingly important. The landmark discovery of Two-dimensional (2D) nanomaterials were first reported with the isolation of graphene in the year 2004 by Andre Geim and Konstantin Novoselov. The 2D materials significantly improve battery and supercapacitors' performance by increasing ion transport, electrical conductivity, and charge storage capacity. Their distinct characteristics make energy storage devices more efficient future applications. Energy storage technology has greatly evolved with the development of 2D nanomaterial preparation for faster charging, higher energy density, and longer lifespans, all of which are crucial in applications like as electric vehicles, renewable energy storage, and portable gadgets. Increased scalability, homogeneity, and cost-effectiveness, synthesis processes have changed over time, moving from early mechanical exfoliation procedures to chemical vapour deposition (CVD) and advanced solution-based technique, synthesis methods have evolved to improve scalability, uniformity, and cost-effectiveness. Future transition and developments in defect engineering and synthesis will further enhance 2D nanomaterials, improving their structural stability, energy density, and conductivity. These developments of Various 2D nanomaterials, including transition metal dichalcogenides, MXenes, phosphorene, boron nitride, and metal-organic frameworks, hold promising potential for energy storage applications propelling the next wave of high-performing and environmentally friendly energy storage technologies.

PP-49

The development of Transitionmetal Dichalcogenides Nanomaterials for Energy Storage Application

Hariharan Subramanian Vijayapriya[a], Jason Thamizhakaran Stanley[b], Amudha Thanarasu[a], Shanmuga Sundar Saravanabhavan[c], Sathya Selva Bala Vasanthakumar[d], Jacklien Emema Rose T.J. [b], Jeny Rachel Biju[b], Baskaralingam Palanichamy[e], Sivanesan Subramanian[b*]*

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Abstract

A supercapacitor is an energy storage device that stores energy. It has greater power density, rapid charging and discharging, long cycle life, and is commonly used in applications like renewable energy systems, hybrid vehicles, and electronics. Pseudocapacitors, which store energy through fast surface redox reactions using materials like metal oxides or conductive polymers and Hybrid Supercapacitors, which combine EDLC and pseudocapacitor properties, such as lithium-ion capacitors, to achieve higher energy and power densities. Flexible supercapacitors are used to power devices like smartwatches, foldable phones, and health monitors. They are needed for the future because they are lightweight, durable, and can bend without breaking. They charge quickly, last longer than batteries, and support renewable energy systems. Transition metal dichalcogenides (TMDs) are materials made from metals like molybdenum or tungsten and elements like sulfur or selenium. They are prepared using methods such as chemical vapor deposition, mechanical or liquid exfoliation, hydrothermal synthesis, chemical mixing, vapor deposition, or electrochemical processes. Flexible supercapacitors using transition metal dichalcogenides (TMDs) offer high power density, rapid charging, and durability, making them ideal for wearable electronics and energy systems. While they face challenges like lower energy density and scalability, their potential in next-gen devices and renewable energy is promising.

PP-50

Nickel Cobaltite Based Nanomaterial for Energy Storage Application

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Abstract

The development of nickel cobaltite ($NiCoO_4$) nanomaterials is made possible by a variety of synthesis techniques, such as hydrothermal, sol-gel, and green synthesis approaches. These nanomaterials are becoming attractive candidates for energy storage applications because of their distinctive spinel structure ($NiCo_2OH_4$ -specific capacitance 687 F/g) on further heat treatment resulting in $NiCo_2O_4$ (at 120 ^{0}C for 2 hours). High electrical conductivity, and remarkable redox activity, which make them appropriate for advanced super-capacitors and lithium-ion batteries. However, issues like structural deterioration and volume expansion during cycling must be resolved. $NiCoO_4$ (specific capacitance 733 F/g) hybridization with other materials, nanostructure optimization, and the use of AI/ML for predictive performance modelling are potential future developments. By combining these tactics, energy storage technologies like batteries and supercapacitors would be more effective, robust, and scalable which satisfy the needs of contemporary technology. Its conductivity and stability can also be increased by combining $NiCoO_4$ with carbon-based materials like graphene($NiCo_2O_4$+GO) or carbon nanotubes ($NiCo_2O_4$/CNTs) or conductive polymers. Another interesting avenue is the creation of wearable and flexible energy storage devices based on $NiCoO_4$. To enhance surface qualities and prevent structural deterioration, advanced coating methods including atomic layer deposition can also be used. As the significance of renewable energy sources increases, effective storage technologies will play an ever-more-important role. These type of nickel cobaltite based advance and innovative materials will be developed more quickly through industry-academia collaboration, guaranteeing their economic viability and environmental sustainability.

PP-51

The 2D Nanoarchitectures for Potential Application for Hybrid Supercapacitors

Muthu Subramanian[a], Jason Thamizhakaran Stanley[b], Amudha Thanarasu[a], Shanmuga Sundar Saravanabhavan[c], Sathya Selva Bala Vasanthakumar[d], Jacklien Emema Rose T.J. [b], Jeny Rachel Biju[b], Baskaralingam Palanichamy[e], Sivanesan Subramanian[b*]*

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Abstract

2D nanoarchitectonics have emerged as a groundbreaking approach for advancing hybrid supercapacitors, owing to their distinctive structural and electrochemical properties offering exceptional potential for various energy applications. Strategically designed 2D materials like graphene, MXenes, and TMDs offer high surface area, tunable functional groups, and excellent conductivity, boosting energy and power densities. These materials facilitate efficient ion adsorption, rapid charge transfer, and minimal ion diffusion paths, making them highly suitable for electrochemical energy storage applications. The morphological versatility of 2D nanoarchitectures, such as layered structures, nanoflakes, and hierarchical designs, enhances electrolyte penetration and ion accessibility, contributing to high capacitance and long cycling stability. Functionalization with heteroatoms (e.g., N, S, P) or the formation of hybrid composites with nanoparticles (e.g., metal oxides and sulphides) introduces synergistic effects, combining electric double-layer capacitance with pseudocapacitance. The versatile applications of 2D nanoarchitectonics extend across energy storage systems, electric vehicles, smart grids, IoT devices, wearable electronics, backup power systems, and aerospace technologies. The integration of advanced electrolytes, such as ionic liquids or solid-state gels, further broadens the voltage window and ensures operational stability. Scalable fabrication techniques like chemical vapor deposition and hydrothermal synthesis enable large-scale deployment, making 2D nanoarchitectures a cornerstone for next-generation energy storage solutions. This work underscores the potential of 2D nanoarchitectonics as a transformative platform for developing high-performance, sustainable, and multifunctional hybrid supercapacitors

PP-52

The Evolution of 2D Mxene for Supercapacitor Application from Origin to Current Trend

Swathi Velmurugan[a], Jason Thamizhakaran Stanley[b], Amudha Thanarasu[a], Shanmuga Sundar Saravanabhavan[c], Sathya Selva Bala Vasanthakumar[d], Jacklien Emema Rose T.J. [b], Jeny Rachel Biju[b], Baskaralingam Palanichamy[e], Sivanesan Subramanian[b*]*

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Abstract

2D MXenes, a family of transition metal carbides, nitrides, and carbonitrides, have gained significant attention in the field of energy storage, particularly for supercapacitor applications. Since their discovery in 2011, MXenes have demonstrated unique properties such as high electrical conductivity, tunable surface chemistry, large specific surface area, and excellent hydrophilicity, making them ideal materials for high-performance supercapacitors. The initial synthesis of MXenes relied on selective chemical etching of MAX phases using HF or other fluoride-containing solutions which are highly toxic. Over time, advanced etching methods, such as minimally toxic etchants and electrochemical exfoliation, were developed. Researches on MXene-based supercapacitors focused on exploring their intrinsic properties and optimizing their electrochemical performance. While pristine MXenes provided impressive capacitance due to their metallic conductivity and surface redox activity, challenges such as restacking, poor cycling stability, and limited oxidation resistance restricted their practical use. Recent advancements have addressed these issues through various strategies, including surface functionalization, ion intercalation, and the design of hierarchical architectures. Additionally, hybrid composites combining MXenes with conductive polymers, carbon-based materials, and metal oxides have shown remarkable improvements in energy density, rate capability, and durability. Furthermore, scalable and environmentally friendly production methods are being explored to facilitate industrial applications. MXenes have also been integrated into flexible and wearable supercapacitors, demonstrating their versatility in next-generation energy storage technologies.

PP-53

2D Nanomaterials for Bone Regeneration

Babita Kumari[a], Jason Thamizhakaran Stanley[b], Shanmuga Sundar Saravanabhavan[a], Amudha Thanarasu[c], Sathya Selva Bala Vasanthakumar[d], Jacklien Emema Rose T.J. [b], Jeny Rachel Biju[b], Baskaralingam Palanichamy[e], Anuradha Dhanasekaran[f], Sivanesan Subramanian[b*]*

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Abstract

The complexity involved in the coordinated action of multiple cell type result in the growth factors leading to bone regeneration. The bone regeneration is a process of repair or replacement of bone tissues and/or new bone. Convoluted complexity with biomaterials two dimensional(2D) nanomaterials have emerged as promising candidates for bone regeneration due to their unique physical, chemical and biological properties. This recent advances in the development of 2D nanomaterials for bone regeneration not limited to graphene's, transition metal dichalcogenides (TMDs) and hexagonal boron nitride (h-BN). The effects of 2D nanomaterials on osteogenesis, angiogenesis and immune responses as well as their potential applications in bone tissue engineering are to be dealt with greater understanding. Advancement in 3D printing, Nanotechnology with Allografts and Scaffolds holds for exploitation of 2D nanomaterials for application in bone regeneration.

PP-54

Target Drug Delivery using 2D Nanomaterials

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Abstract

Drug delivery involves the methods and technologies used to transport and release therapeutic substances in the body effectively. The recent advancements in 2D nanomaterials have shown great pledge for drug delivery operation. The 2D Nanomaterials are constantly explored for drug delivery due to their large surface area and capability to load a variety of drugs, including hydrophobic descent. Recent researches are concentrated on perfecting the targeted delivery of drugs to specific tissues and tackling the biological natural walls using 2D nanomaterials (e.g.- the blood, brain barrier). Advanced hybrid nanomaterials are being developed to increase the therapeutic efficacy by complexing various material properties. 2D nanomaterials for drug delivery must be biocompatible with high surface area, easy of functionalization for various medical treatments. Targeted delivery of drug are made feasible with multimodal and precise control of target specific cells. The graphene is the widely studied 2D nanomaterial and still there are considerable developments in this 2D nanomaterial engineering space for targeted drug delivery. MXenes and transition metal based transition metal dichalcogenides can be a potential drug carrier for targeted drug delivery with enhanced drug loading, surface area, therapeutic science and controlled release of drugs. The developments in 2D nanomaterials for drug delivery application will lead to push the boundaries and hope for new and toxic reductant treatment.

PP-55

2D Nanomaterials for Tissue Engineering Application

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Abstract

Tissue engineering is a biomedical engineering discipline that combines biology and engineering to create tissue outside the body. It's a branch of regeneration medicine that uses cell transplantation. Tissue engineering can be used to repair tissue within the body or to create tissues to replace damaged organs. Tissue engineering has developed into a powerful tool for repairing and reconstructing damaged tissue and organs tissue engineering scaffolds play a vital role in tissue engineering as they not only provide structural support for targeted cell but also serve as templates that guide tissue regeneration and control the tissue structure. 2D Nanomaterials have shown great promise in the field of tissue engineering due their unique physicochemical properties and excellent biocompatibility. These materials can be used to construct scaffolds that provide structural support for cell and guide tissue regeneration. Some of the most commonly used 2D nanomaterials in tissue engineering include graphene, graphene oxide and carbon nanotubes recently. 2D nanomaterials are important in tissue engineering because they provide high surface area for cell attachment are biocompatible, offers strong mechanical properties enable electrical conductivity for never and influence stem cell differentiation for tissue regeneration, neural regeneration and bone regeneration. The development of novel 2D nanomaterials with potential tissue engineering application addressing toxicity, material scalability and long-term stability with the human system is to be explored.

PP-56

Dynamic Modelling and Optimization of Lead Ion Removal Using Reinforcement Learning Approaches

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Abstract:

Lead has become a common contaminant in the water supply systems due to which a need is felt to invent effective removal techniques. This research offers the opportunity to apply reinforcement learning to enhance lead ion removal from aqueous solutions with the aid of adsorption techniques. In this work, we used a magnetic reduced graphene oxide based nickel ferrite nanocomposite as the adsorbent and carried out a detailed study of the impact of the operation parameters such as initial concentration of the dye, the amount of the adsorbent, contact time, pH, and temperature. An environment is created and designed based on OpenAI's Gym in which the simulated fabrication process is encompassed with real-time reinforcement learning algorithms. The findings here presented prove that this combined approach also improves the predictive modeling of the lead ion removal, and brings the overall removal efficiency to as much as 99.86% at the best conditions. The current work can be viewed as a progress in the development of efficient technologies for water treatment as well as a valuable foundation for further studies of environmentally friendly technologies.

Keywords:

Reinforcement Learning, Water Purification Techniques, Lead Ion Removal Techniques, Proximal Parameter Optimization, Neural Network.

PP-57

Synthesis of Sophorolipids from Starmerella bombicola MTCC 1910 using Palm Oil

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Abstract

Bio surfactants (Microbial Surface-Active Agents) have become recently an important product of biotechnology for industrial and medical applications. The reason for their popularity, as high value microbial products, is primarily in their specific action, low toxicity, relative ease of preparation and widespread applicability. They can be used as emulsifiers, de-emulsifiers, wetting agents, spreading agents, foaming agents, functional food ingredients and detergents in various industrial sectors such as Petroleum and Petrochemicals, Organic Chemicals, Foods and Beverages, Cosmetics and Pharmaceuticals, Mining and Metallurgy, Agrochemicals and Fertilizers, Environmental Control and Management, and many others. The present work investigates the synthesis of sophorolipids using palm oil. The availability of vegetable oils is abundant compared to other substrates. In countries like India where vegetable oils are extensively produced and used, economically it is cheaper to employ them as substrates for the production of high value bioproducts.

In the current study sophorolipids was synthesized using Starmerella *bombicola* MTCC1910 with three different oil substrates and the amount of glycolipids from each substrate was quantified and relationship between oleic acid content and the product formed was defined. The amount of sophorolipids obtained was directly proportional to the oleic acid percentage in the oil used. Structural analysis of the product obtained was done using FT-IR spectroscopy and the spectra proved that the glycolipids from *Starmerella bombicola* were lactonic sophorolipids.

PP-58

Anti-Aging Characterisation of Clay Nanotube Formulation

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Abstract:

Collagenase, an enzyme responsible for the degradation of collagen, plays a significant role in maintaining skin health and structure. However, excessive collagenase activity accelerates collagen breakdown, leading to wrinkles, loss of elasticity, and other visible signs of aging. Reducing collagenase activity is crucial for preserving skin integrity and delaying the aging process. Anti-aging formulations, particularly those targeting collagenase inhibition, aim to mitigate these effects by preserving collagen levels and promoting youthful skin characteristics. This study explores the anti-aging potential of clay nanotube-based formulations by assessing their collagenase inhibitory properties. In vitro techniques were employed to evaluate the formulations, offering a controlled and reproducible method for testing enzyme inhibition. Also, in vitro methods are more ethical and cost-effective, as they do not involve live animal or human testing. This approach is considered superior as it eliminates variability associated with in vivo methods, ensuring accurate and consistent results. Nine formulations were tested, categorized into three groups tailored for specific skin concerns: oily, dry, and sensitive skin. Each group consisted of three different combinations, compared against pure Epigallocatechin Gallate (EGCG) as the positive control. Among the oily skin formulations, Sample 3 exhibited the highest collagenase inhibition, outperforming the other two. For sensitive skin, Sample 2 showed superior activity within its group. In the dry skin category, Sample 1 demonstrated the most effective collagenase inhibition. These findings highlight the potential of clay nanotube-based formulations to address specific skin concerns while providing anti-aging benefits. In vitro evaluation stands out as a precise and effective method for assessing enzyme inhibition, ensuring high reliability in results. Its application in this study demonstrates its value in advancing anti-aging research without ethical constraints.

PP-59

Synthesis of Titanium Dioxide Nanotubes and Investigation of their Antibiofilm and Drug Loading Capacity

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Abstract:

Titanium dioxide nanotubes (TNTs), made through anodization, have special properties that make them useful for medical applications, such as improving implant compatibility, perform antibacterial activities and delivering drugs. TNTs were created using titanium foils, and the effect of different electrolyte concentrations (low, medium, and high) on their structure was studied using contact angle measurement and SEM analysis. The analysis showed that the medium concentration electrolyte produced the most uniform nanotubes. Measurements of contact angles revealed that more hydrophilic TNTs, were better at resisting biofilm formation. The TNTs were further examined using scanning electron microscopy (SEM) to confirm their nanotube structure. Tests showed that the TNTs could resist biofilm formation and efficiently load and release drugs, that makes them a promising option for controlled drug delivery. The quality of TNTs can be enhanced by optimizing the electrolyte concentration, anodization voltage, and duration.

PP-60

Development of Integrated Multi-Trophic Aquaculture (IMTA) Systems for Enhancing Coastal Resilience, Nutrient Recovery and Circular Economy

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Abstract:

Integrated Multi-Trophic Aquaculture (IMTA) is a new concept of sustainable aquaculture, characterized by combining species from different trophic levels to produce symbiotic systems that maximize the use of resources, enhance bioremediation, and contribute to the circular economy. This research shall design innovative IMTA frameworks suitable for promoting coastal resilience and sustainability through the ecological and economic benefits of coastal aquaculture. The key components include co-culturing finfish, shellfish, and macroalgae to efficiently utilize organic and inorganic wastes to reduce eutrophication and enhance water quality. Nutrient-rich waste from fed species such as fish is captured and transformed into valuable biomass by extractive species like seaweeds and filter-feeding shellfish. Case studies, including IMTA systems demonstrate significant improvements in nutrient recirculation, with bioremediation efficiencies exceeding 80% and reductions in greenhouse gas emissions. Such findings underscore the role of IMTA in addressing climate change impacts while supporting economic diversification through high-value aquaculture products. It looks into the socio-economic benefits of IMTA: improved employment for coastal communities, reduction of market risks through product diversification, and promotion of sustainable livelihoods. Governance challenges, policy alignment, and socio-cultural acceptance will be addressed in a manner that it provides actionable frameworks for scaling up IMTA in the coastal regions around the world. This study indicates a multi-disciplinary approach of technological innovation, ecological insights, and policy interventions would be needed to establish IMTA as the cornerstone of the blue economy. IMTA furthers sustainable food systems, improves coastal resilience, and fosters economic inclusivity aligned with the global Sustainable Development Goals- by promoting circularity in coastal aquaculture.

PP-61

Fabrication of Wearable Thermoelectric Generators using Antimony Sulfide (Sb_2S_3) Nanostructures

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Abstract:

Thermoelectric technologies are utilized in many industries to convert the generated heat into electricity and vice versa. This project will illustrate how waste heat can be used in converting the same into a useful form of energy, thus enhancing efficiency besides creative solutions. The applications extend into energy harvesting, wherein thermoelectric generators are incorporated into wearable devices, smart clothing, and IoT sensors, where body heat, environmental thermal energy, or industrial waste heat is converted for self-sustaining power. This work aims to make a wearable thermoelectric generator using antimony sulfide (Sb_2S_3) nanostructures known for their high quality and superior thermoelectric power with photoconductivity. Sb_2S_3 is preferred over others because of its high-power conversion from heat into electricity, ideal for wearable devices producing energy. The method used to synthesise is hydrothermal and is based on $SbCl_3$ and Na_2S in the presence of $CO(NH_2)_2$ prepared at 120, 160, 200, and 240 °C for 12 hours. This method is ecologically friendly, scalable, and cost-effective and aimed at wearable thermoelectric generator applications. This research underscores the potential of Sb_2S_3 nanostructures in the realm of wearable thermoelectric applications, presenting a viable option for sustainable energy harvesting.

PP-62

Copper Oxide/Functionalized Multi-wall Carbon Nanotubes: Catalyst in Action for Efficient Organic Dye Degradation

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Abstract:

The degradation of dyes is a tedious task due to their tenacious and stable nature. Dye-contaminated water can cause severe health issues to humans, animals, and aquatic species. The removal of dyes from contaminated water systems necessitates efficient and eco-friendly degradation methods. In the present study, copper oxide/functionalized multi-wall carbon nanotubes (CuO/F-MWCNTs) nanohybrid was synthesized. The synthesized nanohybrid was characterized using X-ray diffraction (XRD) for structural analysis, scanning electron microscopy (SEM) for morphological analysis, and Fourier transform infrared spectroscopy (FTIR) for functional group identification. The synthesized nanocomposite was used as a catalyst for the degradation of organic dyes Rhodamine B (RhB), p-Nitrophenol (PNP) and mixture of these two dyes in the presence of sodium borohydride ($NaBH_4$). The degradation efficiency was evaluated by monitoring the changes in dye concentration over time using UV-Vis spectroscopy. The results demonstrated that the CuO/F-MWCNTs composite exhibited remarkable catalytic activity in degrading RhB, PNP and mixture of these dyes under optimized conditions.

Keywords: CuO/F-MWCNTs, Rhodamine B, p-Nitrophenol, Catalytic activity.

PP-63

Studies On Catechol Oxidase Catalytic Activity of Mesoporous Co(II) Schiff Base Complex

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Abstract

Cobalt(II) dithiocarbazate-silane complex [3APTES+AQSMDTC@Co(II) complex] was synthesized using a newly developed Schiff base (SB) ligand derived from acenaphthoquinone (AQ), S-methyldithiocarbazate (MDTC), and (3-aminopropyl)triethoxysilane (3APTES), together with cobalt(II) acetate salt. The mesoporous cobalt(II) complex [MCM 41@AQSMDTC@Co(II) complex] was fabricated by MCM 41 on the cobalt(II) dithiocarbazate-silane complex. The new confirmation of the complex was extensively characterized using various analytical techniques. FT-IR was used for functional group analyses, and SEM-EDX and TEM were utilized to evaluate surface morphology, elemental composition, particle size distribution, and oxidation status. PXRD was employed to determine crystallinity, while physicochemical parameters and thermal stability of the resulting MCM 41@AQSMDTC@Co(II) complex were determined using nitrogen absorption-desorption measurements and TGA, respectively. Additionally, the heterogeneous catalyst was monitored for catecholase (Cat-ox) activity using UV-vis spectroscopy, which involves the conversion of 3,5-di-tert-butylcatechol (3,5-DTBC) to 3,5-di-tert-butylquinone (3,5-DTBQ). The mesoporous cobalt(II) catalyst could be recovered and reused without significantly losing its catalytic ability.

Keywords: S-methyldithiocarbazone ligand; Cobalt(II) silane complex; MCM 41; Mesoporous catalyst; Catechol oxidase.

PP-64

Sol-Gel Derived Zinc Aluminate: A Pathway to Wireless Applications

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Abstract

Researchers are now investigating suitable dielectric materials to meet the demand for miniaturized and lightweight wireless microstrip patch antennas. Nanoparticles of zinc aluminate ($ZnAl_2O_4$) have a low loss and a high dielectric permittivity, making them ideal for use in microwave applications. This paper details the chemical composition, morphology, structural and dielectric properties of $ZnAl_2O_4$ nanoparticles synthesized using a sol-gel technique. Crystallinity of the prepared nanoparticles was 19.5 nm for ZnO wurtzite. Further, we measure the dielectric permittivity at 30, 40 and 50 °C, with results of 8.82, 8.80 and 8.78 respectively. With recorded values of dielectric loss were 0.06, 0.04 and 0.05, the prepared nanoparticle was found to decrease with increasing frequency.

Keywords: Gahnite, Sol-Gel Process, Dielectric Permittivity, Dielectric Loss.

PP-65

Sustainable Methanol Production From Activated Sewage Sludge Using Two-Stage Anaerobic Digesters Biogas With Membrane-Fortified Purification

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Abstract

The two-stage configuration enhances volatile solids reduction, increases methane yields, and supports hydrogen co-production in the initial phase. The biogas is purified through a membrane-fortified system to remove impurities such as carbon dioxide (CO_2), hydrogen sulfide (H_2S), and water vapor. The highly selective membranes ensure efficient methane enrichment while minimizing energy losses. Purified methane undergoes catalytic reforming, producing syngas (CO and H_2) under controlled conditions. The syngas is subsequently converted into methanol via a thermochemical synthesis process, leveraging advanced catalysts for high selectivity and yield. This integrated approach not only valorizes sewage sludge into a renewable fuel but also reduces greenhouse gas emissions and mitigates environmental pollution from waste streams. Furthermore, the use of membrane technology ensures cost-effective and energy-efficient biogas upgrading compared to conventional methods. This study highlights the potential of coupling advanced anaerobic digestion and membrane purification systems for sustainable methanol production. The proposed framework aligns with circular economy principles, enabling energy recovery from waste while fostering a cleaner, greener future.

Keywords: Sustainable methanol production, activated sewage sludge, two-stage anaerobic digestion, membrane technology, catalytic reforming

PP-66

3D Bio-Printed Scaffolds for Bone Regeneration Using Natural Polymers

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Abstract

Recently, 3D bio-printed scaffolds emerged as the novel transformative approach toward bone regeneration that merges advanced additive manufacturing techniques with natural biocompatible polymers. This research addresses the fabrication and utilization of bio-printed scaffolds of sodium alginate and k-carrageenan in terms of extracellular matrix-mimicking design that facilitates healing for bone tissues. The intrinsic properties of natural polymers, such as biodegradability, non-toxicity, and cellular compatibility, are utilized to enhance the structural integrity and bioactivity of these scaffolds. The scaffolds are fabricated using 3D printing technology with precise control over pore size, porosity, and mechanical strength to ensure a balance between cellular ingress and structural stability critical for bone tissue engineering. The sodium alginate incorporation confers hydrogel-like characteristics, thus enabling cell adhesion and proliferation, whereas k-carrageenan improves the mechanical strength and ionic cross-linking of the scaffold, making it even more bioactive. These scaffolds are specifically designed for repairing critical bone defects, where they will allow vascularization and osteogenesis through an interconnected porous network. Micro-CT, histomorphometric analysis, and immunolabeling have shown that these scaffolds successfully support the deposition of bone matrix proteins, differentiation of osteoblasts, and trabecular bone formation. This approach greatly improves over traditional methods of scaffold fabrication, in that it surpasses the difficulty faced in attempting to replicate native bone's intricacies and functionalities. The printed constructs also appear promising for their potential to offer custom designs toward specific patients' anatomy, therefore lessening complications at the post-operative period. The compatibility between natural polymers and 3D printing technology presents an adaptive platform that offers great possibility toward tissue engineering in an environment-friendly and clinically significant orthopedic application.

PP-67

Manganese Molybdate Nanomaterial Used for Crystal Violet Dye Degradation

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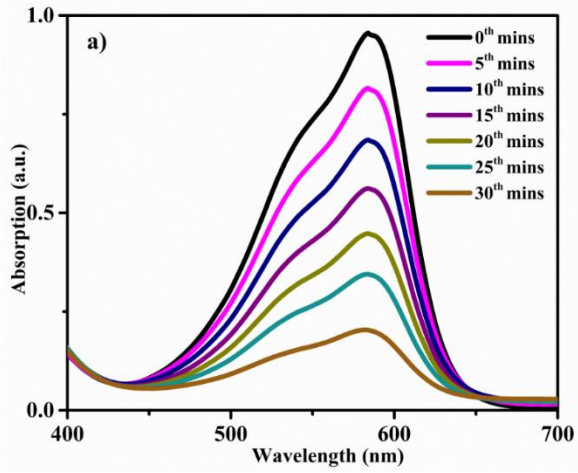
Abstract

Wastewater contamination remains a pressing environmental issue globally. To address this challenge, $MnMoO_4$ nanomaterial is synthesized using a microwave-assisted method for the degradation of organic pollutants in wastewater. This material exhibits remarkable properties, including tunable band structures, environmental friendliness, cost-effectiveness, high surface area, and adjustable electrical conductivity. Comprehensive characterization of the synthesized $MnMoO_4$ is conducted using PXRD to confirm crystalline structure, FE-SEM with EDS for morphological and elemental analysis, FT-IR for functional group identification, and BET measurements to evaluate its specific surface area. Additionally, XPS provides qualitative and quantitative insights into the elemental composition and chemical states. The photocatalytic performance of $MnMoO_4$ is evaluated through the photodegradation of crystal violet dye under ultraviolet light illumination, achieving an impressive degradation efficiency of 91%. These findings highlight the potential of $MnMoO_4$ nanomaterial used as an effective photocatalyst for removing organic pollutants from wastewater.



UV-Visible spectra of the photocatalytic crystal violet dye degradation.

PP-68

Biocompatible Thiol protected Iron Nanoclusters $Fe_n(SR)_m$ for Photochemical Sensing of Cu^{+2} ions.

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Abstract

Metal nanoclustes (2-10 nm) fill the gap between discrete metal atoms and plasmonic nanoparticles, they show novel quantum-size effects and precise structure-property correlations at the atomic level. These homo-metal nanoclusters due to their unique properties is exploited in applications like sensing, catalysis and fabrication of energy storage devices. In this study, a Bio-compatible ligand- Glutathione, protected Iron nanocluster $Fe_n(SR)_m$ is synthesised for precise photochemical sensing of Cu^{+2} ions. Cu^{+2} ions are essential biological element of our body and are associated with neurodivergent diseases. The homeostasis of the said ion in the human body due to concentration retention of copper in higher level of food chain is directly linked to kidney damage, Parkinsons disease and other malignancies. Though existing methods like absorption spectrometry, electrochemical methods do exist, photochemical sensing is facile, inexpensive and quick in detecting the Cu^{+2} ions. Thus, the $Fe_n(SR)_m$ prepared was isolated via PAGE (Polyacralyamide gel electrophoresis) and was characterised using UV-Visible Spectroscopy, Photoluminescence, Dynamic Light Scattering, and FT-IR studies. The $Fe_n(SR)_m$ nanocluster will further be characterised using SEM, HR-TEM and Mass spectrometry to find its composition with atomic precision. Then achieved nanoclusters will be employed for photochemical sensing application of Cu^{+2}.

Key words: Fe NCs- Cu^{+2} ion sensing- photochemical detection- Biocompatible nanocluster.

PP-69

Ultrastable Heterocyclic Thiolate-Protected Nickel Nanocluster Crystals for Catalysis and Electrochemical Sensor Applications.

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Abstract

Nanoclusters are small mighty structures with sizes less than 10 nm. Thiolated protected metallic nanoclusters are tiny intricate nanoscopic particles that are conflunced by several staple motifs. Atomically precise structures have scaled down to sizes less than 2nm. These structures exhibit quantum confinement with wider HOMO-LUMO and thus they are no longer metallic they tend to behave like molecules. Nanoclusters' opto-physical and chemical characteristics are counterintuitive to their metal due to a greater band gap from the fermi level. These properties enable them to be employed in semiconductors, sensors, energy conversion, and conservation applications. Herein we have protected ultastable Ni nanoclusters with a heterocyclic thiolate ligand 3-mercapto-benze-imidazole by wet chemical method. MBI is a dimeric, and an anticorrosive stabilizer. Azole ligands have enhanced antifungal properties, are biocompatible, and are thermodynamically stable thus they act as a capping and protecting agent on Ni metal. Ni precursor was reduced using a mild reducing agent like NaOH and synthesis was swift. NiMBI clusters were then crystalized by seeding with a suitable solvent. The nanoclusters were found to be in sizes <10 nm, which pertains to discrete energy levels observed, quantum confinement effects, and higher surface-to-volume ratio when compared to their bulk counterpart. The obtained crystals were characterized using UV-visible spectroscopy, spectrofluorometer, DLS, XRD, and TEM and would be further extended to applications like chemical remediation, optoelectronics, biosensing, anti-corrosion, and photosensitization studies.

PP-70

Iron oxide nanoparticle core-shell magnetic microspheres: Applications toward targeted drug delivery

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Abstract

This study describes a sensitive reactive oxygen species (ROS)-responsive lecithin (LEC) incorporated iron oxide nanoparticle (Fe_3O_4 NP) system with potent anti-inflammatory properties and even more so when the antioxidant drug curcumin (CUR) is encapsulated in the PLGA hybrid magnetic microsphere system (Fe_3O_4@LEC-CUR-PLGA-MMS). The delivery system is responsive to ROS including an H_2O_2 environment to release the payload (CUR) drug. Greater cytotoxicity properties were observed in the presence of Fe3O4@LEC-CURPLGA-MMS against A549 and HeLa S3 cells with IC_{50} values after 24 h of 10 and 12 µg/mL and 10 and 20 µg/mL, respectively. The present Fe_3O_4@LEC-CUR-PLGA-MMS system demonstrated much better in vitro cytotoxicity, cellular morphological changes and moreover an ability to limit colony formation for A549 and HeLa S3 cancer cell lines than non-cancerous cells, and thus, should be further studied for a wide range of medical applications.

Key words: Poly (D, L-lactide-co-glycolic acid); Lecithin; Magnetic core microsphere; Cytotoxicity; Targeted drug delivery

PP-71

PVP-Assisted Fe_2O_3 Nanomaterial for Methylene Blue Photocatalytic Degradation

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Abstract:

Water pollution caused by organic contaminants is a critical environmental concern. Addressing this issue, Fe_2O_3 nanomaterial was synthesized via a polyvinylpyrrolidone (PVP)-assisted hydrothermal method, demonstrating potential for wastewater treatment applications. Detailed material characterization was performed using powder X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), Fourier transform infrared spectroscopy (FT-IR), and X-ray photoelectron spectroscopy (XPS). The photocatalytic performance of Fe_2O_3 was evaluated through the degradation of methylene blue dye under ultraviolet (UV) light irradiation. Within just 120 minutes, the material achieved an impressive degradation efficiency of 91%, demonstrating its rapid and effective pollutant breakdown capabilities. This study underscores Fe_2O_3's efficacy as an eco-friendly photocatalyst for removing organic pollutants from wastewater.

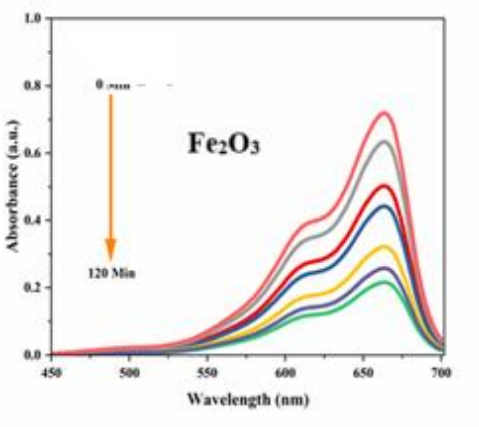

Figure 1. UV-Visible spectra for the photocatalytic degradation of crystal violet dye.

PP-72

Low Dose (mGy) Indirect Conversion X-Ray Sensors Based on $Cs_3Cu_2I_5$ and $CsPbBr_3$ Coated BPW-34 Photodiode

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Abstract

Halide semiconductors have demonstrated tremendous applicability in optoelectronic research owing to their fascinating functional properties. Cesium Copper Iodide ($Cs_3Cu_2I_5$) and Cesium Lead Bromide ($CsPbBr_3$) have been utilized in numerous applications like photovoltaics, photodetectors, and scintillation detectors. Both the materials were synthesized by solid-state exchange reaction, dissolved in dimethyl formamide (DMF) and mixed with PVDF polymer then coated onto the top surface of the photodiodes as thick films. The photocurrent characteristics of $Cs_3Cu_2I_5$ and $CsPbBr_3$ indirect X-ray sensors, upon exposure to X-rays at 70 kVp energy under various X-ray exposures and zero bias conditions, were recorded. Both materials exhibit significant response to the incident X-rays. These experimental findings explore the possibility of using both the materials for produce low-dose indirect conversion x-ray sensors. These results will be discussed in detail with suitable mechanisms.

PP-73

Exploring the Role of p-n Junctions in Catalytic Efficiency of TiO_2 for Solar-Driven Hydrogen Evolution

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Abstract:

Constructing a p-n heterojunction using TiO_2/M-X embedded with C-M effectively addresses low photocatalytic efficiency caused by rapid electron-hole recombination and limited visible light absorption. This research utilized a simple wet impregnation method to prepare nanocomposite, with X-ray diffraction (XRD) confirming the phase purity of TiO_2 and M-X respectively. Diffuse reflectance spectroscopy (DRS-UV) and Brunauer-Emmett-Teller (BET) surface area analysis indicated that optimized concentrations of M-X and C-M significantly improved visible light absorption and increased the surface area of TiO_2. The alignment of band edges between TiO_2 and M-X promoted effective charge transfer, facilitated by the internal electric field at the p-n heterojunction interface. The presence of C-M further enhanced charge carrier transport and accelerated surface redox reactions. Analyses using electron paramagnetic resonance (EPR), photoluminescence (PL) and electrochemical impedance spectroscopy (EIS) revealed defect sites and improved charge transport efficiency within the composite. Under direct sunlight, the TiO_2/M-X/C-M photocatalyst achieved an impressive hydrogen evolution rate of 8979 μ mol h^{-1} g_{cat}^{-1}, surpassing pristine TiO_2, M-X, and the binary TiO_2/M-X nanocomposite. This outstanding performance is attributed to the precise loading of M-X and C-M, which enhanced charge separation and light harvesting. A Z-scheme mechanism was proposed to elucidate the photocatalytic activity, supported by band edge potential calculations and PL/EIS studies that confirmed improved efficiency for hydrogen generation under solar irradiation. This work underscores the potential of the TiO_2/M-X/C-M composite for solar-driven hydrogen production.

Keywords: H_2 evolution; Photocatalysts; p-n heterojunction; TiO_2; Water splitting.

PP-74

A Review on Application of Uio-66 MOF And Its Composites for Future Prospects

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Abstract:

UiO-66, a zirconium-based metal-organic framework, is gaining attention due to its high surface area, tunable porosity, and good thermal and chemical stability. It can be synthesized via solvothermal, hydrothermal, Microwave-assisted or solvent-free mechanical grinding methods. Solvothermal synthesis is widely recognized as a technique that produces particles with highly crystalline nature. however, the hydrothermal method is more eco-friendly. Microwave-assisted synthesis accelerates reaction times, whereas solvent-free mechanical grinding is sustainable but slower. Direct synthesis using zirconium alkoxides is costly but ensures high-purity UiO-66 . UiO-66 and its composites find versatile applications across diverse fields, showcasing their remarkable potential and adaptability. Magnetic UiO-66-NH_2 composites are effective in removing pharmaceutical contaminants like salicylic acid (SA) and acetylsalicylic acid (ASA) from water. Chitosan/UiO-66 composites exhibit superior dye adsorption, particularly for methyl orange removal. High surface area in UiO-66 makes it suitable for carbon capture through efficient CO_2 adsorption, while composite materials enhance stability and capacity. In hydrogen storage, carbon nanotubes incorporation improves efficiency, and thus UiO-66 is promising for energy applications. Catalysts based on UiO-66 composites facilitate reduction and organic transformations and optimize catalytic activity. Besides, UiO-66 composites are applicable in gas sensing, water purification, and electrochemical devices like supercapacitors, taking advantage of their tunable properties and functionalization potential. Overall, UIO-66 and its composites are set to play a key role in sustainable energy, environmental, and industrial applications.

PP-75

Fluorescence quenching of benzimidazole derivative with ZrO_2 nanoparticles

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Abstract

New benzimidazole has been designed, synthesized and characterized by spectral studies. Binding interaction studies of benzimidazole with zirconia nanoparticles have been carried out by absorption and fluorescence spectral studies. Benzimidazole is adsorbed on the surface of zirconia nanoparticles through azomethine nitrogen. Fluorescence quenching has been observed due to electron transfer between benzimidazole and zirconia nanoparticles. The conduction band energy position determines the electron transfer from excited state mercapto benzimidazole to zirconia nanoparticles. Based on photo-induced electron transfer mechanism, fluorescent quenching has been explained and apparent binding constant has been calculated.

PP-76

Microsphere $CaMoO_4$/AC heterogeneous structures for supercapacitor application

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Abstract

In this study, a $CaMoO_4$/AC heterostructure composite was synthesized using a simple hydrothermal method to evaluate its electrochemical properties for energy storage applications. The composite, combining $CaMoO_4$ with bio-derived activated carbon (AC) from onion peels, showed enhanced charge storage capabilities. The material was characterized using techniques such as XRD, FTIR, FESEM, XPS, BET, and EDAX, which confirmed its structural integrity and surface composition. As a supercapacitor electrode, the $CaMoO_4$/AC composite exhibited excellent performance with a specific capacitance of 716.58 F/g at 1 mA/cm² and displayed remarkable cycling stability, retaining 94.42% of its initial capacitance after 2000 cycles. The hydrothermal process played a key role in controlling the structure and enhancing the crystallinity of the material, contributing to its improved electrochemical properties. With high capacitance, stability, and the use of sustainable bio-derived materials, this CaMoO4/AC composite emerges as a promising candidate for future energy storage applications, especially in the development of eco-friendly supercapacitors.

PP-77

Redefining The Nanomaterial Nanoarchitectonics for The Development of Self-Assembled Biomass Derived Carbon Architecture

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Abstract

The use of biomass derived carbon is limited and to exploit its fullest potential new and improved approach is needed. In this work, the authors would like to propose a strategy for the development of self-assembled carbon nanoarchitecture with help of Nanoarchitectonics concept. The Nanoarchitectonics is a concept involving classical supramolecular chemistry, materials science and biological science for the development of advanced functional nanomaterials. The self-assembled superstructures are reported and holds a great interest in the material and synthesis science for fabrication and discovery of novel materials with distinct characteristic properties. Previously, reported nanostructures like fullerenes and fullerene-based assemblies, carbon nanotubes (CNTs), graphene and graphene based materials and carbon quantum dots (CQDs) are some of the nanomaterials which had impacted the science and technology for varied applications. This constructive conceptualisation of biomass derived nanoassembly will redefine the nanomaterial science and engineering with potential in energy storage to biomedical applications. The exploitation of biomass derived superstructures with defined morphology will be the material of future. The exploration of a new material space begins here!

PP-78

Green Chemical Synthesis of Rhamnolipid-Capped Silver Nanoparticles for Antimicrobial and Antifungal Applications

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Abstract

Biosurfactant-based rhamnolipids have gained significant attention in medical, pharmaceutical, and food packaging industries due to their antibacterial and antifungal properties. This study synthesizes rhamnolipid-capped silver nanoparticles (AgNPs) via sunlight irradiation, eliminating the need for conventional reducing and stabilizing agents like sodium borohydride. The objective is to develop an eco-friendly, cost-effective synthesis method while evaluating the physicochemical properties and antimicrobial potential of AgNPs. Silver nanoparticles were synthesised by irradiating a mixture of rhamnolipid (0.02M) and silver nitrate (0.01M), with the pH adjusted to 9 using 0.1N NaOH, under sunlight exposure. Nanoparticle formation occurred within 10 minutes, confirming an efficient and sustainable approach. UV-Vis spectroscopy identified an SPR peak at 432 nm, while HRTEM analysis revealed a uniform morphology with an average particle size of 7 nm. DLS and zeta potential measurements confirmed stability, and the critical micelle concentration (CMC) was determined to assess rhamnolipid self-assembly in the nanoparticle solution. The antimicrobial and antifungal efficacy of the synthesized AgNPs was evaluated using well-diffusion and minimum inhibitory concentration (MIC) assays against common pathogens. The results demonstrated significant inhibition zones, confirming strong antimicrobial activity. This study establishes rhamnolipid-capped AgNPs as a sustainable alternative to conventional antimicrobial agents, offering effective microbial control for applications in medical, pharmaceutical, and food packaging industries.

PP-79

Fabrication of Wearable Thermoelectric Generators using Antimony Sulfide (Sb_2S_3) Nanostructures

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Abstract

Thermoelectric technologies are utilized in many industries to convert the generated heat into electricity and vice versa. This project will illustrate how waste heat can be used in converting the same into a useful form of energy, thus enhancing efficiency besides creative solutions. The applications extend into energy harvesting, wherein thermoelectric generators are incorporated into wearable devices, smart clothing, and IoT sensors, where body heat, environmental thermal energy, or industrial waste heat is converted for self-sustaining power. This work aims to make a wearable thermoelectric generator using antimony sulfide (Sb_2S_3) nanostructures known for their high quality and superior thermoelectric power with photoconductivity. Sb_2S_3 is preferred over others because of its high-power conversion from heat into electricity, ideal for wearable devices producing energy. The method used to synthesise is hydrothermal and is based on $SbCl_3$ and Na_2S in the presence of $CO(NH_2)_2$ prepared at 120, 160, 200, and 240 °C for 12 hours. This method is ecologically friendly, scalable, and cost-effective and aimed at wearable thermoelectric generator applications. This research underscores the potential of Sb_2S_3 nanostructures in the realm of wearable thermoelectric applications, presenting a viable option for sustainable energy harvesting.

PP-80

Highly Improved heterogeneous metal-organic framework heterostructure for photocatalytic degradation of organic contaminants

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Abstract:

The remediation of organic pollutants in wastewater is a crucial issue for human health and environmental integrity. Heterogeneous catalysis has emerged as a leading technology for the cleanup of volatile organic compounds (VOCs), owing to its environmental sustainability and operational simplicity, despite the known ecological risks associated with these molecules. Metal-Organic Frameworks (MOFs) are formed by the combination of organic and inorganic linkers, resulting in materials with high porosity. According to current research, inorganic connectors are metal centers that can exist alone or in clusters, whereas organic linkers are organic entities that have two or more functional groups that allow for coordination interactions with metal centers. In this study, we produced MOF/Metal nanocomposites that were then investigated using UV-DRS, FT-IR, XRD, FE-SEM, HR-TEM, BET, PL and XPS methods. Innovative wastewater treatment procedures make use of advanced oxidation/reduction processes (AO/RPs).

Keywords: Metal-organic framework; metal nanoparticles; Organic pollutants.

PP-81

Synthesis of Freestanding PPy/Ni_3S_2 Hybrid Electrodes from Ni Foam and Diverse Sulfur Sources for High-Performance Asymmetric Supercapacitors

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Abstract

The development of well-constructed asymmetric supercapacitors with high energy density has garnered significant attention. In this study, we report for the first time to our knowledge a novel approach to energy storage through the incorporation of polypyrrole (PPy) onto a binder-free Ni_3S_2 hybrid electrode, fabricated via a simple hydrothermal method. The binder-free composite electrode effectively shortens ion diffusion pathways and enhances conductivity. The optimized electrode demonstrates a predominantly pseudocapacitive behavior, driven by redox mechanisms arising from synergistic interactions between its multiple oxidation states and composite structure. This enhanced electrode delivers an impressive specific capacitance of 1470 F/g at 1 A/g and exhibits exceptional stability, retaining 78.94% of its capacitance and achieving a Columbic efficiency of 99.5% after 15,000 cycles. Furthermore, when integrated into an asymmetric supercapacitor a specific capacitance of 100 F/g at 1 A/g was achieved corresponding to an energy density of 74.9 Wh/kg at a power density of 1356.4 W/kg, with a high capacitance retention of 91.7% after 10,000 cycles. These findings offer a promising strategy for developing advanced energy storage systems.

Keywords

Ni_3S_2, PPy, supercapacitor, binder free, high energy density ASC, Energy storage

PP-82

Effect of Manganese Doping NiO Materials as an Efficient Electrode for Enzyme-Free Glucose Sensor Applications

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Abstract

Pure and Mn-doped NiO (NiO/Mn@NiO) nanomaterials were synthesized by the simple chemical precipitation method. The various characterizations have been made on synthesised materials and prepared electrode for the non-enzymatic glucose sensor applications. Initially, the material structure and their functional groups were confirmed by the Powder X-ray diffraction (PXRD) and Fourier Transform Infrared (FTIR) spectroscopy analysis respectively. The squared like morphology has been obtained and their elemental composition were examined by the Field emission scanning electron microscopy (FESEM) along with energy-dispersive X-ray spectroscopy (EDX). The absorbance of prepared materials has been examined by UV-Vis-NIR spectroscopy. The electrochemical properties of NiO/Mn@NiO were investigated and characterized using Cyclic Voltammetry (CV) and resultant its performance is more compatible for electrochemical applications. NiO/Mn@NiO exhibits the good electrochemical activity that includes glucose detection sensitivity of 524 μA $mM^{-1}cm^{-2}$ & 3853 μA $mM^{-1}cm^{-2}$ and detection limit of 0.357 mM & 0.326 mM respectively with linear range of 0.5 mM to 2.5 mM. The Mn@NiO NP shows the better electrocatalytic activity than the pure NiO NP. The results show the proposed doping nanomaterials can be promising candidate for glucose sensing applications.

PP-83

Synthesis and Characterization of Titanium Dioxide Nanotubes and Investigation of their Surface for Possible Antibiofilm Property

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Abstract:

Titanium dioxide nanotubes (TNTs) have special properties that make them useful for medical applications, such as improving implant compatibility, perform antibacterial activities and delivering drugs. TNTs were fabricated through anodization process, titanium foils, and the effect of different electrolyte concentrations (low, medium, and high) on their structure. The electrolyte used consisted of glycerol, ammonium fluoride (NH_4F), and deionized water. Tube formation was studied using contact angle measurement and scanning electron microscopy (SEM) to confirm their nanotube structure. Measurements of contact angles revealed that the medium concentration shows more hydrophilic TNTs than other concentration, were better at resisting biofilm formation. The SEM analysis showed that the medium concentration electrolyte produced good formation of nanotubes but not uniformly. Further optimization of electrolyte ratios, anodization voltage and duration are necessary to achieve uniform tube formation and enhance the overall quality of TNTs which is effectively useful in biomedical applications.

PP-84

Binding interaction of substituted benzimidazole with ZnO nanoparticles

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Abstract

Binding interaction studies of substituted benzimidazole with ZnO nanoparticles have been carried out by absorption and fluorescence spectral studies. Substituted benzimidazole is adsorbed on the surface of ZnO nanoparticles through azomethine nitrogen. Fluorescence enhancement has been observed due to electron transfer between substituted benzimidazole and ZnO nanoparticles. The conduction band energy position determines the electron transfer from excited state substituted benzimidazole to the ZnO nanoparticle. Based on photo-induced electron transfer mechanism, fluorescent enhancement has been explained and apparent binding constant has been calculated. The antimicrobial effect of the non-functionalized and functionalized ZnO nanoparticles dispersed in water was investigated.

PP-85

DFT and Molecular Docking Studies of DMPC lipid bilayer with Aspirin

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Abstract

Density Functional Theory (DFT) is a quantum mechanical method used to study the electronic structure of molecules and materials. In this, the phospholipid like DMPC, DFT is employed to understand their electronic properties, interactions, and chemical reactivity at an atomic level. Aspirin (acetylsalicylic acid, $C_9H_8O_4$) is a widely used nonsteroidal anti-inflammatory drug (NSAID) with analgesic, antipyretic, and anti-inflammatory properties. It also has antiplatelet effects, making it useful for cardiovascular disease prevention. The Molecular docking studies of Aspirin with DMPC lipid bilayer shows excellent binding affinity, finds potential application in biological studies and computational chemistry. Molecular Electrostatic Potential (MEP) of DMPC represents the electrostatic potential created by the charge distribution of a molecule in three-dimensional space. Mulliken charge distribution of DMPC helps understand the charge transfer, molecular reactivity, and intermolecular interactions. Frontier molecular orbitals (FMOs) and play a key role in chemical reactivity, charge transfer, and optical properties. The energy gap (ΔE) determines molecular stability and reactivity. Time-dependent DFT (TD-DFT) and Emission spectra can be used to study electronic excitations and emissive nature in lipid environments.

PP-86

Harnessing the potential of UU 200/Bi_4O_8nanocomposite to optimize energy efficiency in supercapacitor and electrocatalysis application

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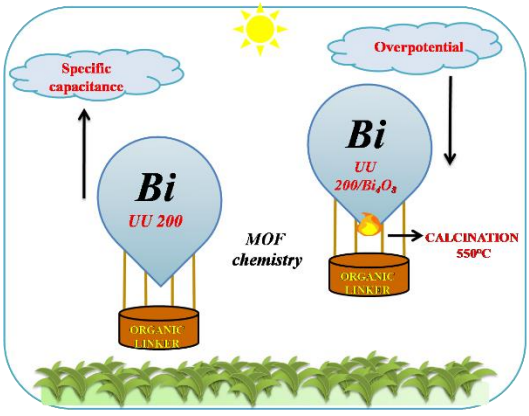
Abstract

In the quest for solution of sustainable energy, the focus is on advancing efficient energy storage systems and production of green hydrogen. In this work, UU 200 (UU: Uppsala University) metal-organic framework (MOF)/bismuth oxide (Bi_4O_8), termed the UU 200/Bi_4O_8 nanocomposite, has been synthesized and used as an electrode material for supercapacitor applications and an electrocatalyst for hydrogen evolution reaction (HER). XRD, Raman, FT-IR, and XPS tests showed that the UU 200/Bi_4O_8 nanocomposite was successfully formed. The SEM and TEM images revealed that the UU 200/Bi_4O_8 nanocomposite exhibits a mixed rod and spherical structure. The supercapacitor performance of pure UU 200 and UU 200/Bi_4O_8 nanocomposite has been examined through cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance (EIS) measurements. Interestingly, the UU 200/Bi_4O_8 nanocomposite delivered a maximum specific capacitance value of 220 F g^{-1} at 1 A g^{-1}. Furthermore, the UU 200/Bi_4O_8 nanocomposite potential was extended beyond its energy storage capability to the electrocatalytic HER process. The electrocatalytic HER performances were assessed through linear sweep voltammetry (LSV), CV, chronoamperometry (CA), and EIS analysis. The overpotential (η) of 130 mV and the Tafel slope value of 131 mV dec^{-1} indicate the UU 200/Bi_4O_8 nanocomposite supremacy in advanced applications. The UU 200/ Bi_4O_8 nanocomposite electrode has excellent supercapacitor and water-splitting performance, allowing it to acquire green energy for future energy needs.

Material	Specific capacitance (F g^{-1})	b-value	Overpotential @10 mA cm^{-2}	Tafel slope (mA dec^{-1})	C_{dl} (mF cm^{-2})
UU 200	46	0.57	150	131	6
UU 200/Bi_4O_8	220	0.44	130	142	11



PP-87

Towards Efficient CO_2 Reduction: TiO_2-based Photocatalysis and Adsorption Mechanisms

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Abstract

As global warming accelerates, finding effective ways to tackle CO_2 emissions has never been more urgent. The idea of converting CO_2 into valuable materials is not only a sustainable way to reduce atmospheric pollution but also offers promising economic opportunities. In search for these solutions, researchers are focusing on materials that can address both environmental and economic challenges. One such material is TiO_2, a widely studied semiconductor known for its photocatalytic properties. Our study explores how TiO_2's performance in CO_2 reduction is shaped by its synthesis method and structure. It is found that the specific surface area and the interactions between TiO_2 and the products of the reaction are key to its efficiency. It is discovered that anatase, one of TiO_2's phases, is more effective than others in the photocatalytic reduction process, likely because it absorbs visible light more efficiently—an essential trait for harnessing solar energy for CO_2 conversion.

PP-88

A theoretical investigation employing DFT and molecular modeling was conducted on Acyclovir Surface-Enhanced Raman Scattering (SERS) utilizing silica nanocomposites that are loaded with silver, gold, and platinum.

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Abstract:

Acyclovir (ACV) presents a valid treatment option for COVID-19. Currently, there are 705 million confirmed cases of the coronavirus disease (COVID-19) globally, resulting in over 7 million fatalities. Acyclovir (ACV) serves as one therapeutic choice for COVID-19. This antiviral medication is used to treat herpes, chickenpox, and shingles, and it falls within the class of antiviral drugs. It inhibits the replication of the virus within human cells, preventing the production of new viruses and aiding in the resolution of the infection. Recent advancements in medicine have made it possible to deliver drugs using nanocages. The medical sector has employed drug delivery systems utilizing nanocages. We examined how the antiviral drug ACV adsorbs on Au/Ag/Pt…SiO_2-loaded silica nanocomposites, which are associated with the B3LYP/LANL2DZ basic set through DFT. We applied the Frontier Molecular Orbital (FMO) concept of Molecular Electrostatic Potential (MEP) to identify the active site of the molecule. According to the bioactivity evaluation, both the molecule and its complexes demonstrate strong drug-like characteristics and comply with Lipinski's rule of five. A comparative analysis was performed between the biological properties of organic molecules and nanometal clusters. We also explored the Localized Orbital Locator (LOL) and Electron Localization Function (ELF) of ACV when combined with nanocomposites. The UV-Visible spectra of the compounds were analyzed employing the TD-DFT method in both polar protic solvents (ethanol, methanol, and water) and polar aprotic solvent (DMSO). Additionally, Acyclovir (ACV) was docked with the chosen proteins and assessed through molecular docking.

PP-89

Magnetic iron oxide nanoparticles@lecithin/poly (l-lactic acid) microspheres for targeted drug release in cancer therapy

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Abstract

The use of targeted chemotherapy is a promising solution to mitigate the side effects and dosage of drugs. This research focuses on the development of magnetic microspheres (MMS) based drug carriers for targeted chemotherapy, formulated with iron oxide nanoparticles (Fe_3O_4 NPs) and poly (l-lactic acid) (PLA) loaded with the antibiotic drug Ciprofloxacin (CIF). In this study, Fe_3O_4 NPs were synthesized using pomegranate peel extract as a natural reducing and stabilizing agent. The double emulsification method (W1/O/W2) was employed to produce Fe_3O_4@LEC-CIF-PLA-MMS, which were characterized using various spectral and microscopic techniques. The drug encapsulation efficiency for Fe_3O_4@LEC-CIF-PLA-MMS was found to be 80.7 %. The in vitro drug release of CIF from Fe_3O_4@LEC-CIF-PLA-MMS induced by H_2O_2 and GSH- stimuli was found to be 87.55 % and 82.32 %, respectively in acidic pH 4.5. Notably, the magnetically triggered drug release behaviour of Fe_3O_4@LEC-CIF-PLA-MMS (93.56 %) was assessed in acidic pH environment upon exposure to low-frequency alternating magnetic field (LF-AMF). Fe_3O_4@LEC-CIF-PLA-MMS demonstrated significantly enhanced in vitro cytotoxicity (IC50 = 0.8 ± 0.03 µg/mL) against the HeLa-S3 cancer cell lines. Nevertheless, these research findings highlight the potential of Fe_3O_4@LEC-CIF-PLA-MMS for further development as a chemotherapeutic agent and hold promise for the future of targeted cancer treatment.

PP-90

Synthesis, characterisation and biological evaluation of tyramine derived Schiff base ligand and its transition metal (II) complexes

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Abstract:

In this study, a new tyramine derived Schiff base ligand (L) (L=1,3-phenylenebis-4-aminoantipyrinyl-4-aminoethylphenol) and its derived transition metal(II) complexes $[Cu(L)Cl_2]$(1), $[Ni(L)Cl_2]$(2), $[Co(L)Cl_2]$ (3) and $[Zn(L)Cl_2]$ (4) have been synthesized and well characterized by the way of different spectroscopic and analytical techniques. Analytical and spectroscopic studies result suggests that metal(II) complexes more probably have octahedral geometry. DNA binding tendency of L and metal(II) complexes 1-4 have been assessed by probing their ability to bind with Calf Thymus DNA (CTDNA) via electronic absorption and cyclic voltammetry titration methods. The results clearly reveal that the metal(II) complexes may interact with DNA through intercalation mode of binding and their binding constant value K_b was found to be in the range of 11.2 – 23.7 $\times 10^5$ M^{-1}. The DNA damage study has also been investigated by gel electrophoresis technique. Interestingly, it was found that all the complexes could cleave the circular plasmid pBR 322 super coiled (SC) DNA efficiently in the presence of activators. The complexes showed enhanced antifungal (MIC, 2.7 – 6.9 µg/mL) and antibacterial (MIC, 3.1 – 3.9 µg/ mL) activities compared to the free ligand.

PP-91

Polyurethane (PU) resin for effective adsorption of heavy metal: Artificial intelligence and machine learning approach

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Abstract

The properties of polymers have drawn a lot of interest in their use in heavy metal removal. Nevertheless, the traditional approach of applying polyurethane (PU) resin substance by trial and error is labor-intensive and time-consuming. Using machine learning (ML) and artificial intelligence (AI) has the potential to significantly increase the effectiveness of polyurethane resin with the necessary qualities. Here, five different AI/ML models were used for the first time to forecast certain polyurethane resin characteristics, including cation exchange capacity (CEC), which is essential for heavy metal adsorption. This research mainly focuses on the utilization of Support Vector Regression (SVR), Decision Tree Regression (DTR), Linear Regression (LR), and Gaussian Process Regression (GPR) models to PU adsorption studies. Prior research has concentrated on the relationships between PU resin's CEC and application performance; however, no study has directly predicted the adsorption capacity (qe) of heavy metals from PU resin. With a predicted qe of around 0.65 mmol/g for Arsenic III, for example, DTR model was successfully offered the best way to produce PU resin with the highest qe. The study of the adsorption mechanism confirmed the dominant role of cation exchange, demonstrating the great potential of such different AI/ML models to support the production of designer PU resin. Finally, the experimental verification of the optimum solution revealed that the adsorption capacities of the as-produced optimum PU resin were similar to the ones predicted by the AI/ML model (validation R^2 0.878).

Keywords: Heavy metal, adsorption, polyurethane resin, Artificial intelligence, Machine learning.

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Prediction of N-doped graphene/$NiWO_4$ visible light photocatalyst in rhodamine-B degradation based on machine learning

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Abstract:

Examining the impact of N-doped graphene/$NiWO_4$ visible light photocatalysts on the experimental variables during rhodamine-B degradation may facilitate the identification of optimal parameter combinations to enhance degradation efficiencies overall. Experimental approaches have been shown to be an excellent option for assessing the entire experimental process, but they have the drawbacks of being expensive, time-consuming, and potentially prone to instrumental mistakes. These issues can be avoided with machine learning techniques. Five conventional machine learning models—Linear Regression (LR), Decision Tree (DT), Support Vector Machine (SVM), Random Forest (RF), and Gradient Boosting (XGB)—were examined for their efficacy in predicting the rhodamine-B degradation efficiencies of the N-doped graphene/$NiWO_4$ photocatalyst. XGBoost (XGB) had the highest reliability, with R^2, RMSE, and MAE values of 0.973, 3.985, and 2.685, respectively. Additionally, the relevance of features was ranked using the SHAP approach and XGB's feature importance in order to make the results interpretable. This work introduced a novel concept for the development of N-doped graphene/$NiWO_4$ photocatalysts aimed at the degradation of rhodamine-B, as well as intelligent algorithms for forecasting the photocatalytic efficacy of these materials.

Keywords: N-doped graphene/$NiWO_4$, Photocatalyst, rhodamine-B, Machine learning, XGBoost