



Abstracts:

PHYSICAL SCIENCES

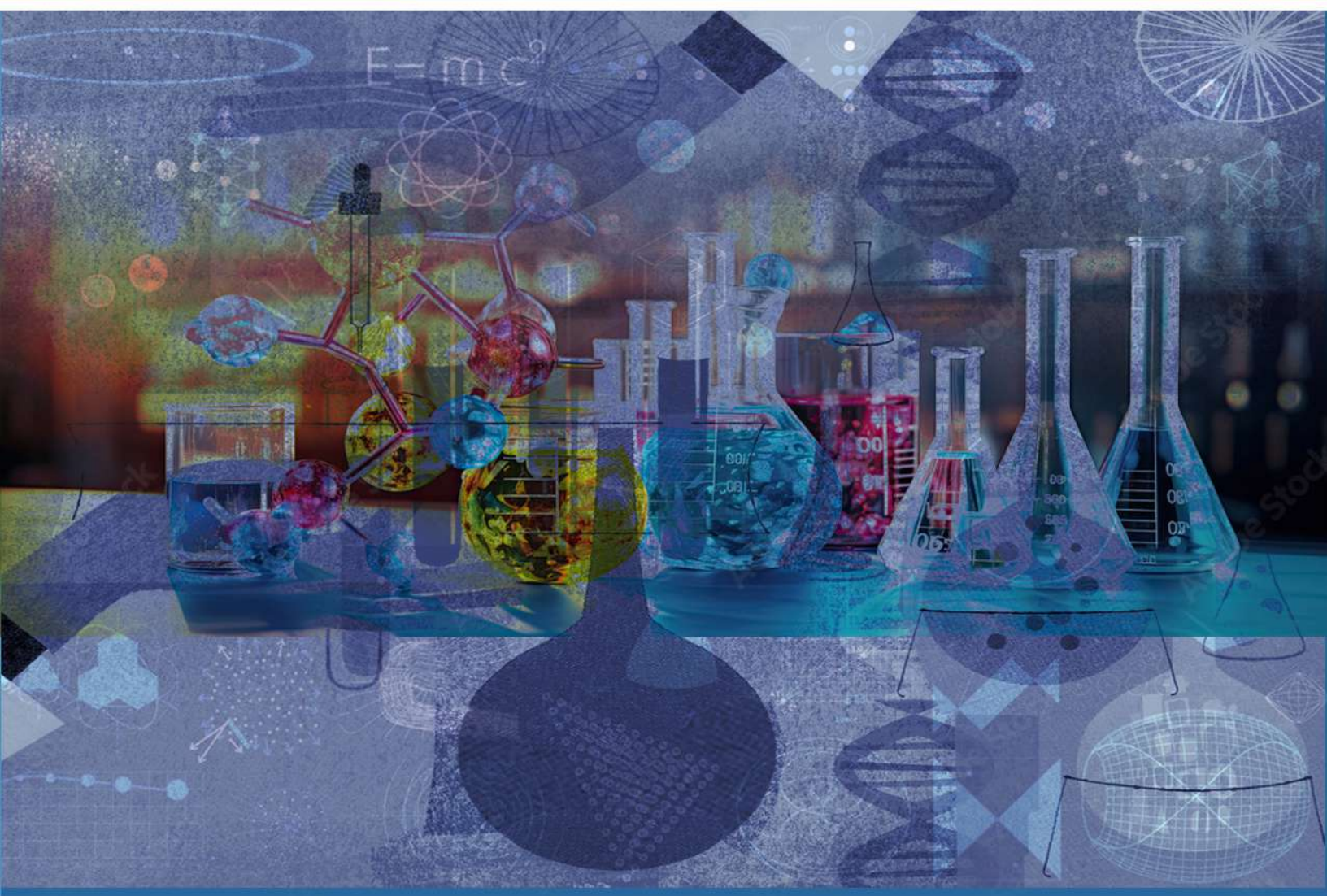
94th Annual Session of NASI and Symposium

on

“Accelerated R & D towards a *Viksit Bharat*”

at

IISER Bhopal



Abstracts
(Physical Sciences)
94th Annual Session of NASI and
Symposium
on
“Accelerated R & D towards a
***Viksit Bharat*”**

Dedicated to the Past President of the Academy
Bharat Ratna Dr. M.S. Swaminathan

December 01-03, 2024

Hosted by



Indian Institute of Science Education and Research (IISER)
Bhopal - 462066



94th Annual Session of NASI and Symposium on Accelerated R & D Towards a Viksit Bharat

jointly organized by

The National Academy of Sciences, India (NASI)

&

Indian Institute of Science Education & Research Bhopal (IISERB)

dedicated to the Past Presidents of the NASI,

- Bharat Ratna, Prof M. S. Swaminathan
- Padma Bhushan, Dr Manju Sharma

on 1-3 December 2024

at

IISERB, Bhopal Bypass Road, Bhauri, Bhopal, Madhya Pradesh, INDIA

---Tentative Programme ---

Day 1: December 1, 2024 (Sunday)

Children Science Meet (10:30 am - 12:00 pm) Venue: L-5

Local Coordinator: Prof Abhijit Patra, IISER Bhopal

Chairman	Prof Ajoy K Ghatak <i>Past President, NASI; Former Professor of Physics, IIT Delhi</i>
Co-Chair	Prof Snigdha Thakur Dept of Physics, IISER Bhopal
Resource Person	<ol style="list-style-type: none">1. Prof Ajoy K Ghatak, Formerly Professor of Physics, IIT Delhi (25 + 5 min) Title: Einstein, $E = mc^2$ & The Atom Bomb2. Padma Shri Prof H.C. Verma, Formerly Professor of Physics, IIT Kanpur (50 + 10 min) Title: Learning Physics from Nature and Scoring in Exams

Lunch (12:45 - 2:00 PM)

Venue: Dining Hall, VH

REGISTRATION: LHC (11:00 AM - 2:00 PM)

December 1, 2024 (Sunday)

Inaugural Session (2:15 pm - 03:30 pm) Venue: L- 5 in LHC

Coordinator: Prof Chandan Sahi, IISER Bhopal

✚ To begin with the lighting of the lamp

Welcome (4 min)	Prof Vinod K Singh, IIT Kanpur Convener Prof Sourav Datta, IISER Bhopal Local Co-convener
About NASI (5 min)	Prof Jayesh R. Bellare, IIT Bombay General Secretary (OS), NASI
About IISER Bhopal (6 min)	Prof Gobardhan Das Director, IISER Bhopal
Guest of Honor (6 min)	Dr Shailesh Nayak NIAS Bangalore
Guest of Honor (6 min)	Dr Ajai Chowdhry Founder, HCL; Chairman, EPIC Foundation
President (10 Min)	Prof Balram Bhargava President, NASI
Chief Guest (20 Min)	Dr Jitendra Singh Hon'ble Union Minister of State (Independent Charge) for Science & Technology, Govt of India
Felicitation of the Guests (3 min)	
Vote of thanks (4 min)	Prof Daya Shankar Pandey, BHU Varanasi General Secretary (HQ), NASI, Prof Abhijit Patra, IISER Bhopal Local Co-convener
National Anthem & Group Photographs	

Tea/Coffee 3:30 PM - 4:00 PM (Foyer of LHC)

Session 1: Quantum Research & Futuristic Applications (4:00 PM - 4:50 PM)

Coordinator: Manmohan Kapur, IISER Bhopal Venue: L-5 in LHC

Chair/ Co-Chair	Anurag Sharma, IIT Delhi Akshay Modi, IISER Bhopal
Talk 1 (20 + 4 min)	Ankur Raina, IISER Bhopal <i>Bits to Qubits: Revolutionizing Computing with Quantum Mechanics</i>
Talk 2 (20 + 4 min)	Kasturi Saha, IIT Bombay <i>Quantum Sensing with Nitrogen Vacancy Centers in Diamond</i>

NASI Foundation Day Lecture (4:50 - 5:25 PM) Venue: VH Auditorium

- ❖ **Preside over:** Prof Balram Bhargava, President, NASI
- ❖ **Chairperson:** Prof Ashok Misra, Past President, NASI; JNCASR Bangalore
- ❖ **Speaker :** Dr Ajai Chowdhry, Founder HCL

Session 2: Climate Resilience & Sustainability (5:30 PM - 6:45 PM) Venue: L-5 in LHC

Coordinator: Dhanyalekshmi Pillai, IISER Bhopal

Chair/ Co-Chair	Amit Roy, Vice President, NASI Pankaj Kumar, IISER Bhopal
Talk 1 (20 + 4 min)	Shailesh Nayak, NIAS Bangalore <i>Climate Implications and Action: A Policy Perspective</i>
Talk 2 (20 + 4 min)	Suruchi Bhadwal, TERI New Delhi <i>Understanding Climate Change and its Responses</i>
Talk 3 (20 + 4 min)	Ramya Sunder Raman, IISER Bhopal <i>Atmospheric Aerosol Management to Advance Sustainable Development Goals: Opportunities and Strategies</i>

Dinner 7.30 PM onwards Venue: VH Lawn

Day 2: December 2, 2024 (Monday) Venue: VH Auditorium

Special Lecture (9:00 - 9:20 PM) Venue: VH Auditorium

- ❖ **Chairperson:** Prof Balram Bhargava, President, NASI
- ❖ **Speaker:** Dr Subhra Chakraborty, NIPGR
A Tribute to Madam Manju Sharma - Woman of Wonder

Session 3: Health and Disease: Prevention, Control & Treatment (9:20 AM - 10:10 AM)

Coordinator: Ram Kumar Mishra, IISER Bhopal Venue: VH Auditorium

Chair/Co-Chair	Madhu Dikshit, CDRI Lucknow Paramjit Khurana, <i>University of Delhi</i>
Talk 1 (20 + 4 min)	Amit Prakash Sharma, ICGEB New Delhi <i>Malaria: traversing the tracks between structural biology and epidemiology</i>
Talk 2 (20 + 4 min)	Sanjay Behari, SCTIMST Trivandrum <i>Biomedical device development in contributing to health care in the country: the road map, the successes, and the travails</i>

Tea Break and Poster Visit (10:15 - 10:45 AM)

Session 4: Artificial Intelligence & Machine Learning (10:45 AM -11:55 AM)

Coordinator: Aasheesh Srivastava, IISER Bhopal Venue: VH Auditorium

Chair/Co-Chair	R.S. Verma, MNNIT Allahabad Mitradeep Bhattacharjee, IISER Bhopal
Talk 1 (20 + 4 min)	Manish Gupta, Google India Research & IIT Bangalore <i>Transformative Power of AI and Open Challenges</i>
Talk 2 (20 + 4 min)	Nitin Saxena, IIT Kanpur <i>(Artificial) Intelligence in Society</i>
Talk 3 (20 + 4 min)	Manik Varma, Microsoft Research & IIT Delhi <i>Foundation Retrieval Models: The Next Paradigm Shift in Search, Recommendation & Chat</i>

Session 5: Cyber Security & Data Sovereignty (12:00 PM - 1:10 AM)

Coordinator: Rahul Garg, IISER Bhopal

Chair/Co-Chair	J.P. Mittal, BARC Mumbai Vishal Rai, IISER Bhopal
Talk 1 (20 + 4 min)	Manindra Agrawal, IIT Kanpur <i>Securing Critical Infrastructure of India</i>
Talk 2 (20 + 4 min)	Jayant Haritsa, IISc Bangalore <i>Light on Malicious Database Queries</i>
Talk 3 (20 + 4 min)	Shweta Agrawal, IIT Madras <i>Post Quantum Cryptography: The Road Ahead</i>

Lunch Break (1:15 - 2:20 PM)

Session 6 (Sectional Presidents' Session): (2:25 PM - 3:15 PM) Venue: VH Auditorium

Coordinator: Surajit Saha, IISER Bhopal

Chair/Co-Chair	S.M. Yusuf, BARC Mumbai Gopal C. Kundu, KIIT Bhubaneswar
Talk 1 (20 + 4 min)	S Natarajan, IISc Bangalore Sectional President, Physical Sciences <i>Designing new white light emitting materials for low-cost LEDs</i>
Talk 2 (20 + 4 min)	Ch Srinivasa Rao, ICAR-NAARM, Hyderabad Sectional President, Biological Sciences <i>Net Zero Emission Target by 2070: Agriculture Sector Contributions</i>

Tea Break and Poster Visit (3:15 PM - 4:00 PM)

Council Meeting (3:15 - 5:00 PM)

Venue: VH Boardroom 3

Fellows Meeting (Induction of Newly Elected Fellows; 5:00 -6:15 PM)

Venue: VH Auditorium

Annual General Body Meeting (6:15 - 7:15 PM)

Venue: VH Auditorium

Dinner 7.30 PM onwards

Venue: VH Lawn

Day 3: December 3, 2024 (Tuesday)

Session 7a (Parallel Session: Physical Sciences): (9.00 AM - 9.50 AM)

Venue: VH Auditorium

Coordinator: Nitin Patil, IISER Bhopal

Chair/Co-Chair	S Natarajan, IISc Bangalore (Sectional President, Physical Sciences) Sanjit Konar, IISER Bhopal
Speaker 1 (20 + 4 min)	Joyanta Chaudhury, IISER Bhopal <i>Toward a Carbon-Neutral Energy Economy via Recycling CO₂</i>
Speaker 2 (20 + 4 min)	Arindam Ghosh, IISc Bangalore <i>Designing emergent physics and technology with interfaces</i>

Session 7b (Parallel Session: Biological Sciences): (9.00-9.50 AM)

Venue: Seminar Hall 1 in VH

Coordinator: Apurba L. Koner, IISER Bhopal

Chair/Co-Chair	Ch Srinivasa Rao, ICAR-NAARM, Hyderabad (Sectional President, Biological Sciences) Sourav Datta, IISER Bhopal
Speaker 1 (20 + 4 min)	C.R. Mehta, Central Institute of Agricultural Engineering Bhopal <i>Food Security in India and Farm Mechanization</i>
Speaker 2 (20 + 4 min)	M. Sundaram, ICAR, IIRR Hyderabad <i>Gene Editing. Research and Development in Rice</i>

Tea Break (9:50 - 10:25 AM)

Discussion, Recommendations and Valedictory (10:30 - 12:00 PM)

Venue: VH Auditorium

Coordinator: Saptarshi Mukherjee, IISER Bhopal

Chairperson: Dr Subhra Chakraborty, NIPGR

Remarks (5 min)	Balram Bhargava, President, NASI
Remarks (3 min each)	Council Members, Sectional Presidents, Chairs, Speakers, etc
Felicitations and 'Outstanding Paper Presenters' receive their certificates. (30 min)	
Vote of Thanks (3 min)	Santosh Shukla Acting Exec Secretary, NASI

Lunch & Departure (12.30 - 2.00 PM)

PRESIDENTIAL ADDRESS

Designing new white light emitting materials for low-cost LEDs

by

Prof. Srinivasan Natarajan

Sectional President (Physical Sciences)

94th Annual Session of NASI at Bhopal

Solid State and Structural Chemistry Unit,

Indian Institute of Science,

Bangalore 560012

DESIGNING NEW WHITE LIGHT EMITTING MATERIALS FOR LOW-COST LEDs

Srinivasan Natarajan

Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560012

Email: snatarajan@iisc.ac.in

In recent years, much effort has been expended to develop new hosts for solid-state devices. There are many advantages in developing solid-state light-emitting devices (WLEDs) due to the energy efficiency as well as environmentally benign nature. Two approaches have been adopted towards the development of white LEDs. In the first approach, blue-emitting LEDs such as InGaN, (450–480 nm) in combination with near UV-emitting LEDs and a suitable phosphor can be attempted. In the second approach, the use of UV-LED with tricolor (Red, Green, Blue; RGB) phosphors. Controlling the photoluminescence behavior in the material would require the following considerations: (i) crystal structure needs to be flexible (adaptable) to accommodate different substitutions and (ii) good coupling of activators to host lattice along with efficient energy transfer. Single-phase white-light-emitting phosphors have attracted much attention recently to develop white LEDs. The advantages of this approach are many: (i) good luminescence efficiency and color rendering index; (ii) reproducibility of the luminescence and (iii) easier synthesis, which reduces the manufacturing costs. It may be noted that it is important to realize good energy transfer between the sensitizer and activator in a single-phase phosphor.

Over the years, we have explored many mineral structures towards developing new and interesting compounds. Our studies also indicate that we could successfully develop white-light emission using minimal use of rare-earth ions. We have also been successful in creating white light emission by combining Bi³⁺ ions and rare earths.

References

M.L.P. Reddy et al, *J. Photochem. Photobiol. C: Reviews*: 33, 109–31 (2017)
S.Natarajan et al, *Chemistry – An Asian J*, **2017**, 12,2734; *European. J. Inorg. Chem.*, **2018**, 2277; *Inorg. Chem.*, **2019**, 58, 8560; *Dalton Trans.*, **2020**, 49, 17649; *Chem. Asian J.*, **2020**,15, 3104; *Chemistry A European J*. **2021**, 27, 1995; *Eur. J. Inorg. Chem.*, **2023**, 26, e2023004; *Eur. J. Inorg. Chem.*, **2023**, 26, e202300305. *Chem. Asian J*. **2024**, 19, e202301113; *Chem. Mater.*, **2024**, 36, 5356 – 5369.

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POSTER PRESENTATION

1. SYNTHESIZED SULFOSALICYLIC ACID FUNCTIONALIZED SILVER NANOPARTICLES FOR THE DETECTION OF ARSENIC IONS IN AQUEOUS SOLUTION VIA SURFACE-ENHANCED RAMAN SCATTERING TECHNIQUE

Aarti Jaiswal, Aparna Tiwari and K N Uttam

Saha's Spectroscopy Laboratory, Department of Physics, University of Allahabad, Allahabad

Email: aarti.uoa11@gmail.com

Abstract

For maintaining water quality, planning remediation strategies and ecosystem restoration works, detecting metal ions in aquatic water bodies is critical. Plasmon-enhanced spectroscopy using plasmonic particles tailored and decorated by organic molecules provide promising simple, portable, robust, and economically viable sensing systems for metal ions in the field or point-of-care settings. For this, silver nanoparticles functionalized with sulfosalicylic Acid (SSA-AgNPs) have been synthesized by chemical reduction method for the detection of Arsenic [As (V)] ions in aqueous solution using the Surface-enhanced Raman scattering (SERS) technique. The addition of metal ions to the SSA-AgNPs solution induces alteration in the spectral features of the peaks of SSA-AgNPs. In addition, they also lead to the formation of new characteristic bands. A significant enhancement in the intensity has been observed for these bands in the form of SERS signals. These peculiar characteristic peaks can be used for the detection of As (V) ions in an aqueous solution. The study demonstrates the applicability of SSA-AgNPs as plasmon-enhancing spectroscopy agents for the simple, prompt, easily accessible, and portable tool for the detection of metal ions pollution in an aqueous medium.

2. TO DESIGN SENSOR INTEGRATED PASSIVE MICROSTRIP ANTENNA FOR MEDICAL MONITORING APPLICATIONS

Abhishek Kumar Saroj , Ravi Mali, Praveen Singh Rathore and Manoj Kumar Meshram

Department of Electronics Engineering

IIT (BHU) Varanasi, India 21005

Email: abhisheksaroj1988@gmail.com

Abstract

This article proposes a real-time sensor integrated passive micro strip antenna (SIPMA) for temperature monitor for medical, industrial and defense systems. It works at 433MHz ISM band with SAW (Surface Acoustic Wave) Sensor. In current age of technology, health and healthy life become primary concern. In this article our primary focus to develop smart systems that monitors real time health status and continuously manage or warn if any abnormality detected. It is also used for industrial and defense sector real-time monitoring systems. There is also a major challenge to develop such kind of system that cannot consume power or works in passive environment. So, in this work, a saw sensor based micro strip antenna for medical, industrial and defense applications-based system's monitoring application is proposed that works without any active source i.e. battery less systems. Another novelty of this work is, it is proposed for

frequency (400 00 MHz) ISM Band which is absolutely free for industrial, scientific, and medical sector applications. This SIMPA was design on FR-4 (Flame Retardant) Substrate with dimension $51 \times 28 \times 1.6$ mm³ with dielectric constant 4.4 and $\tan\delta$ is 0.002. SIMPA shows resonating frequency at 434 MHz with band width 32.13 MHz and Gain total of 6.92 dB approximately. Back metal effect is also studied for this proposed structure, which shows not major changes in reflection coefficient. SAW sensor integrated antenna sends passive data through the antenna wirelessly and received by interrogator systems. Interrogator system processed measured data by signal processing and produce composite analysis in terms of temperature, pressure, pH and many more. So, this article presents simulated a low profile compact antenna of size 51×28 mm² integrated with SAW sensor. High Frequency Structured Simulator (HFSS) version 22 is used for the data validation.

3. EFFECT OF SELF ACTIVATED YTA1-XNBXO4 MIXED HOST MATRICES ON DOWNSHIFTING EMISSION AND QUANTUM CUTTING EMISSION FROM EU3+ AND YB3+ IONS: APPLICATION IN FINGER PRINTING AND SOLAR CELL APPLICATIONS

Abhishek Roy, S.B. Rai and K. N. Uttam

Department of Physics, Faculty of Science, University of Allahabad, Prayagraj 211002, INDIA

Department of Physics, Institute of Science, Banaras Hindu University, 221002, INDIA

Email: abhishek_ra2024@allduniv.ac.in , sbrai49@yahoo.co.in & knuttam@rediffmail.com

Abstract

This work investigate the effect of mixed matrices $YNb_{1-x}Ta_xO_4$ on downshifting (DS) and quantum cutting emission (QC) from Eu^{3+} and Yb^{3+} doped phosphors. The Eu^{3+}/Yb^{3+} doped $YTa_{1-x}Nb_xO_4$ (where $x = 0, 0.25, 0.50, 0.75, 1.0$) phosphors have been synthesized by solid state reaction method. The structural and optical properties have been investigated in detail by XRD, SEM, FTIR, UV-Visible absorption and photoluminescence and lifetime measurements. The Eu^{3+} doped $YTa_{1-x}Nb_xO_4$ phosphors shows different $4f-4f$ derived transitions from $5D_0-7F_J$ ($J = 1, 2, 3, 4$) transitions on charge transfer band and 394, 465 nm excitation. The strong DS emission behaviour been further quantified by CIE digram. The DS emission properties have been compared on the basis of assymmetric ratio $I(5D_0 \rightarrow 7F_1)/I(5D_0 \rightarrow 7F_2)$. Moreover, Yb^{3+} doped $YTa_{1-x}Nb_xO_4$ phosphor emit intense near infrared emission from 900-1035 nm region on UV excitation. The intense Downshifting red and strong QC emission in near-infrared region can be utilized in latent fingerprinting and efficiency enhancement in c-Si solar cell.

4. SYNTHESIS AND MOLLUSCICIDAL ACTIVITY OF SOME NOVEL FUSED 2 - ARYLOXYMETHYL - ARYL - THIOXO - [1,2,4]TRIAZOLO - [3,2-B] [1,3,4] - THIDIAZOLE

Abhishek Singh

Department of Chemistry, U. P. College, Varanasi 221002

Email: abhupc@gmail.com

Abstract

Several novel and few fused heterocyclic system viz 2-aryloxymethyl -aryl -thioxo-[1,2,4] triazolo-[3,2-b][1,3,4]-thidiazole(III) have been synthesized from key intermediate 2-amino

- aryloxymethyl-[1,3,4]- thiazole(I). This nucleophilic substitution reaction of (I) with phenylisocyanide in methanol afforded the fused system (III). The structure of intermediate and final compounds have been determined by means of IR, ^1H NMR, mass spectrometry and elemental analysis. All the synthesized compounds have been screened for their molluscicidal activity against the snail *Lymnaea acuminata*.

5. COST EFFECTIVE CHIP FABRICATION TECHNOLOGY

Adhisha Roy and Santanu Talukder

Department of EECS, IISER Bhopal, Bhopal, Madhya Pradesh, India

Email: santanu@iiserb.ac.in

Abstract

The demand for semiconductors is surging as they have become an integral part of every sector from defence to healthcare. The chip dimensions are reducing to meet the industry standards set by Moore's law. The fabrication industry faces increasing costs due to the usage of complex sophisticated lithography systems, thereby driving the need for cost-effective chip fabrication technologies. The semiconductor industry is being set up in India. In this regard, I would like to highlight research and development in the domain of semiconductor fabrication for cost-effective chip fabrication technologies. Strategies like chiplet architectures (system in package) replacing the system on chip (SoC) have paved the way for desirable outcomes with respect to cost, yield, performance, and reliability. Design optimisation and techniques are opted wherein higher efficiency is achieved by design changes and with the reduction in the number of lithographic steps. Non-conventional lithography technique such as scanning probe lithography is actively researched to reduce the mask making cost, multiple patterning is being adopted. Resistless patterning for mask fabrication is another way of cost-effective fabrication. Approaches like effective choice of materials enabling room temperature processing, and integration of artificial intelligence and machine learning into fabrication processes can streamline production, enhancing cost efficiency. By adopting these cost-effective strategies, the semiconductor sector may satisfy rising worldwide demands while preserving its economic viability.

6. MOLECULAR PATHWAYS FOR TECHNOLOGICALLY IMPORTANT COPPER CHALCOGENIDES NANOSTRUCTURES

Adish Tyagi

Chemistry Division, Bhabha Atomic Research Centre Mumbai, India - 400085

Email: tyagia@barc.gov.in

Abstract

Copper chalcogenide nanocrystals (NCs) and their multinary derivatives, which incorporate main-group metals, represent a fascinating class of materials with numerous stable crystal phases. Their unique properties make them highly promising for applications in photovoltaics, thermoelectrics, energy storage, and electrocatalysis. However, to unlock their commercial potential, it is crucial to develop synthesis methods that are efficient, cost-effective, and scalable. One such method is the single-source precursor (SSP) route, which offers significant advantages over traditional solid-state or dual-precursor approaches. The pre-formed bonds between desired elements in SSPs allow for the synthesis of phase-pure materials with high reproducibility and precise control over

size and morphology, especially when combined with appropriate capping agents. Recognizing the technological importance of copper chalcogenides and the versatility of the SSP method, we have focused on utilizing internally functionalized hemilabile chalcogenligand-derived copper complexes as SSPs for synthesizing copper chalcogenide nanostructures. Through a series of experiments, we demonstrated that the choice of precursor plays a critical role in determining the composition and morphology of the final material. Furthermore, the reaction solvent used during thermolysis is pivotal in selectively producing different copper chalcogenide compositions, while also influencing the morphology and optical properties of the nanostructures. Additionally, we emphasize the importance of a molecular core that mimics the final material structure, enabling low-temperature, facile conversion of precursors into nanomaterials. Finally, the potential of these nanostructures has been demonstrated as photon-absorbing materials and as efficient anode materials for lithium-ion batteries, highlighting their broad application potential.

7. GREEN CHEMISTRY APPROACH FOR THE SYNTHESIS OF FE-DOPED MnO_2 NANO PARTICLES AND THEIR ANTIMICROBIAL ACTIVITY

Akanksha Tiwari and Devendra Kumar

Department of Chemistry, Institute of Basic Sciences,

Dr. Bhimrao Ambedkar University, Khandari Campus, Agra 82002

E.mail: akankshatiwari597@gmail.com

Abstract

In the present study a novel plant mediated green method was used to synthesize MnO_2 and Fe-doped Manganese Oxide (MnO_2) nanoparticles by using the leaves extract of *Daturastramonium* as a reducing agent. The synthesized nanoparticles were characterized with the help of FTIR, XRD, HRTEM and FESEM EDAX techniques. The formation of doped NPs was confirmed by visual color change of solution. Crystalline size of doped NPs has been confirmed by P-XRD and HRTEM. Furthermore, Morphology of synthesized NPs was characterized by Field Emission Scanning Electron Microscopy analysis. Antimicrobial activities of nanoparticles were screened for their antibacterial activity in vitro against bacteria *E. coli* and *S. Aureus* and antifungal activity against *A. Niger* and *C. Albicans* by adopting the disk diffusion method. The results of antimicrobial studies exhibited that Fe-doped MnO_2 NPs were very sensitive to antimicrobial pathogens. This new eco-friendly approach of synthesis is a novel, cheap, and suitable technique for large scale commercial production and health related applications of Fe-doped MnO_2 nanoparticles.

8. SYNTHESIS AND ANTIFUNGAL ACTIVITY OF SOME FUSED 2-SUBSTITUTED -[1,2,4]-TRIAZOLO-[3,2-B][1,3,4]-THIDIAZOLES

Akhilesh Singh

Department of Chemistry, K. S. Saket College, Ayodhya- 224001

Email: akhileshchem@gmail.com

Abstract

Several novel and few fused heterocyclic system viz 2-aryloxymethyl -aryl -thioxo-[1,2,4] triazolo-[3,2-b][1,3,4]-thidiazole(III) have been synthesized from key intermediate 2-amino - aryloxymethyl-[1,3,4]- thidiazole(I). This nucleophilic substitution reaction of (I) with

phynylisocyanide in methanol afforded the fused system (III). The structure of intermediate and final compounds have been determined by means of IR, ^1H NMR, mass spectrometry and elemental analysis. All the synthesized compounds have been screened for their antifungal activity against *Colletotrichum falcatum* and *Cephalosporium sacchari*.

9. STRUCTURAL AND MECHANICAL PROPERTIES OF (HALIDE AND OXIDE) CUBIC PEROVSKITES

Amar Kumar

Department of Physics, K. R. (P.G.) College, Mathura, (India), 281001

E-mail: kumarkrc@gmail.com

Abstract

In this paper, semi empirical formula for the structural and mechanical properties of halide and cubic oxide perovskite solids is elaborated in terms of lattice constant (a in Å) and bulk modulus and product of ionic charges of the bonding theory. The evaluation of these properties of new materials, Ionic radii, electronegativity and quantities are very useful parameters and the average ionic radii r_{av} of any compound is key parameter for calculating physical properties. Values of structural properties of the perovskites (halides and oxides) exhibit a linear relationship when plotted against the lattice constant (a°) normalization, but fall on different straight lines according to the product of ionic charges of the compounds. The resulting expressions can be applied to a broad selection of perovskite materials and their properties predictions are in good agreement with the experimental data and those from ab initio calculations.

10. SYNTHESIS AND BIOLOGICAL APPLICATIONS OF INDOLE

Amulya Sinha, Arzoo Siddiqui, Vaibhav Tripathi, Girish Singh, Amit Yadav, Rudraksh Srivastava, Nikhat Fatima, Gautam Kumar, Justin Masih and Vivek Bhaduria

Green Laboratory, Department of Chemistry, Ewing Christian College, University of Allahabad, Prayagraj, Uttar Pradesh, India 11003.

Department of Chemistry, Ewing Christian College, University of Allahabad, Prayagraj, Uttar Pradesh, India 11003.

Email: bvivek17@gmail.com

Abstract

Indoles are ubiquitous in several biologically active compounds of alkaloids, agrochemicals and also pharmaceuticals. The indole ring system is a beneficial structural moiety possessing broad scope of pharmacological attributes like antihistaminic, antifungal, antimicrobial, antioxidant, plant growth regulator, anti-HIV, anticonvulsant, anti-inflammatory as well as analgesic and so on. Indoles belong to the most essential constituents among the heterocyclic frameworks required in the discovery of drug molecules. Thus, the merits of indole substituent fascinated the mind of organic chemists. Indole alkaloids viz. tryptophan are popularly known for their significance in nutrition to animal as well as human being. Serotonin is a significant neurotransmitter observed in animals. Reserpine is incorporated for reducing blood pressure and also utilized as a tranquilizer. The synthesis of indole possessing compounds has drawn attention of several organic as well as medicinal chemists. Analysis of indole chemistry are linked with the formation of indigo dye.

Factually, indole was entitled based on indigo as well as oleum. Transformation of indigo to isatin as well as oxindole broadens the range of synthetic strategies of indole.

11. SENSITIVE AND SELECTIVE DETECTION OF METAL IONS USING 5-SULPHOSALICYLICACID-FUNCTIONALIZED SILVERNANOPARTICLES: A SURFACE-ENHANCED RAMAN SCATTERING APPROACH

Aparna Tiwari, Aarti Jaiswal, and Sweta Sharma

Saha's Spectroscopy Laboratory, Department of Physics, University of Allahabad, Prayagraj, India;

Department of Environmental Sciences, Dr. Harisingh Gour Vishwavidyalya, Sagar, India

Email: aparnatiwari945@gmail.com

Abstract

Organic molecule-tailored Plasmonic nanoparticles show potential as a promising method for fabricating an efficient, uncomplicated, highly sensitive, and selective detection tool. This approach utilizes surface-enhanced Raman scattering (SERS) phenomena that amplifies the Raman scattering from molecules attached to nanostructured metallic surfaces marks a significant milestone in the development of spectroscopic and analytical methods. Further, silver nanoparticle has been synthesized with 5-sulphosalicylic acid (SA-AgNPs) using chemical reduction method and characterize with ultraviolet-visible spectroscopy, X-ray diffraction, and Raman spectroscopy techniques. Syhtesized SA-AgNPs has been used as a probe, for the detection of different metal ions spiked in aqueous solution, by distinctive spectral signatures of metal ions using SERS technique. The carboxyl, hydroxyl, and sulphonyl group attached in 5-sulphosalicylic acid results in the surface modification of silver nanoparticles and provide stability to the synthesized nanoparticles from agglomeration. The SA-AgNPs employed for the identification and quantification of selenium (V) ions in aqueous solutions. The analysis of the Raman signal on addition of SA-AgNPs and metal ions exhibits peculiar Raman bands of the Se (V) that facilitates its detection in water samples. The detection limit and quantification limit are found to be 7.1 μM and 21.7 μM respectively. The acquired Raman characteristics demonstrate the capability of SA-AgNPs to provide an economical, enduring, accessible, user-friendly, precise, and prompt method for identifying Se (V) ion in water-based solutions.

12. ONE-POT SYNTHESIS OF 6- AMINO - METHYL, 4-DIPHENYL, 4-DIHYDROPYRANO [2,3-C]PYRAZOLE –5- CARBONITRILE DERIVATIVES USING NAOH/FLY-ASH IN WATER.

Arvind Kumar Pandey

Department of Chemistry, Model College Rajmahal, Sahibganj, Jharkhand - 814110

Email: drarvindau@gmail.com

Abstract

A series of 6-amino -methyl , 4-diphenyl , 4-dihydropyrano [2, 3-c] pyrazole -carbonitrile derivatives were synthesized by three-component reaction of aromatic aldehydes, malononitrile, and 3-methyl -phenyl -pyrazolin -one using NaOH/Fly ash as catalyst in aqueous media. It has been found that NaOH/fly ash shows efficient catalytic activity in the synthesis. The reaction has the advantages of good to excellent yield, less pollution, low-cost catalyst, ease of separation, and of green reaction pathway.

13. LEAD CANDIDATE IDENTIFICATION USING PYRIDONE-SCAFFOLD AS A RDRPINHIBITOR OF SARS-COV

Ashoke Sharon, Uttam Kumar Mishra, Mika Okamoto and Masanori Baba
Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, India
Center for Advanced Research and Promotion, Kagoshima University, Japan
Email: asharon@bitmesra.ac.in

Abstract

SARS-CoV RdRp modeling, design, synthesis of pyridone scaffold, and SARS-CoV investigation resulted in anti-COVID candidate development. One synthesized novel compound demonstrated comparable activity to Nirmatrelvir (approved protease inhibitor). Molecular dynamic studies on RdRp also validate the experimental result on RdRp. Further, modeling studies show that the hydroxyl amino group (NH-OH) played a significant role in base pairing in RdRp. The pyridone shows $\pi \dots \pi$ stacking with U20 in the primer, and the NH-OH group forms base pairing like the existing drug molecule Molunaparavir with U0 in the template.

The significant biological results reveal the promising discovery of a novel pyridone scaffold as an anti-COVID candidate identification with the RdRp mechanism. The compounds were significantly active with their EC^{50} in the standard and omicron strains and had low cytotoxicity ($CC_{50} > 100 \mu M$). Nirmatrelvir, an approved protease inhibitor, and remdesivir nucleoside inhibitor were used as references for the comparison in this investigation.

The studies using biosafety level 3 (BSL3) facilities on novel small-molecule compounds showed that novel 2-pyridone -carboxylic acid derivatives strongly inhibited SARS-CoV replication in cell cultures. Furthermore, they found that the derivatives are likely to have a distinguished mode of action compared to existing anti-SARS-CoV drugs, such as remdesivir (RNA polymerase inhibitor) and Nirmatrelvir (protease inhibitor).

14. EFFECT OF POPS ON HUMAN HEALTH AND THE ENVIRONMENT IS A GLOBAL ISSUE OF CONCERN.

Ashutosh Singh

K. S. Saket PG College, Ayodhya, 224001 Uttar Pradesh
Email: asinghkssaket@gmail.com

Abstract

The rapid growth in chemical and agrochemical industries during the last century have resulted in the environmental releases of a large number of new chemical compounds into the environment. The daily use of chemicals includes mainly organic synthetic chemicals, and the number increases continuously. Over the last decades, there has been an increasing focus on a subset of harmful organic chemicals, mostly of anthropogenic origin, that are commonly classified as Persistent Organic Pollutants (POPs). Certain organic chemicals are persistent, bio accumulative in the environment for a long time and toxic. These chemicals cause long-term harm to the health of human beings and the planet's environment. Throughout the world, people and their environments are exposed on a daily basis to Persistent Organic Pollutants or POPs. POPs and their effects on human health and the environment is a global issue of concern. They accumulate in animals and humans, predominantly in fatty tissue. As these chemicals move up the food chain they concentrate to levels that are harmful to humans, wildlife and aquatic animals.

15. CHEMOTHERAPEUTIC AND PHOTO-ACTIVE NANOMEDICINES FOR BREAST CANCER MANAGEMENT

Asifkhan Shanavas

Institute of Nano Science and Technology

Sector 81, Mohali, Punjab 140306

Email: asifkhan@inst.ac.in

Abstract

Triple-negative breast cancer (TNBC), is one of the most aggressive form of cancer that has limited options of treatment. Surgery is a primary frontline intervention for breast cancer patients. However, TNBC bears heightened risk of relapse after surgical resection, primarily attributable to its invasive characteristics, limited treatment modalities, and dismal prognosis. This requires adjuvant therapies such as chemotherapy to be followed up. In a typical clinical setting, cancer therapeutic outcome is often enhanced by employing combinatorial strategies involving the co-administration of multiple anticancer drugs for synergistic chemotherapy. However, poor oral availability & aqueous solubility in addition to systemic toxicity limit their potential in the present clinically available forms. All these observations demand development of new generation of therapeutics such as photo-active metal nanoparticles as well as reinforcing the conventional approach like nanoencapsulation of multiple drugs in single formulation. Further, the implementation of regional and localized delivery of active pharmaceutical ingredients has emerged as a strategy to mitigate dose-limited toxicity. We will discuss intravenous, intra-tumoral and intra-operative implantation based drug and metal based therapeutic strategies for management of TNBC in animal models.

16. BIOSORPTION POTENTIAL OF PLANT LEAF POWDER FOR CATIONIC DYE REMOVAL FROM AQUEOUS SOLUTION USING BATCH AND OPTIMIZATION STUDIES

Dheeraj Kumar

Department of Chemistry, K. R. (PG) College, Mathura, UP, India

Email: dchem2107@gmail.com

Abstract

Environmental pollution is an unfavorable alteration of the chemical and physical constitution of the atmosphere by pollutants. Generally, a pollutant is a harmful solid, liquid or gas present in such concentration in the environment which tends to be injurious to all biological and sometimes even the physical species. The effluents containing residual dyes which are not biodegradable has become a serious environmental problem in the last decade due to the increasing and fast-growing usage of dyes in different applications. Even traces of dye in water largely effects the aesthetics and transparency in water bodies. Biosorption is leaded to the decolorizing the waste water by using the agricultural waste through the adsorption technique. The low cost of operation and occurred through the green reaction under the usage of the natural waste is the interested method for the dye removal. In the present study the Crystal violet (CV) adsorption onto Combretum

indicum leaf powder was investigated in terms of both adsorption efficiency and kinetic study. The experimental data were fitted for adsorption isotherm models. Development of mathematical model and its optimization to reduce the complicity of the process. Optimization provides the effect of several investigating factors at various level with their influence on each other. The experimental results showed that the adsorbent has heterogeneous surface activity and the adsorption of dye on it follows pseudo-second order kinetics and the adsorption is spontaneous and exothermic.

17. UNRAVELING EARLY-STAGE DYNAMICS OF IMINE CAGE-TO-COVALENT ORGANIC FRAMEWORK TRANSFORMATION AT LIQUID-LIQUID INTERFACE

G. Shreeraj, Madhvi Tiwari, Arkaprabha Giri, Venkateshwar Rao Dugyala and Abhijit Patra
Department of Chemistry, IISER Bhopal, Department of Chemical Engineering, IISER Bhopal
Email: shreeraj20@iiserb.ac.in, vdugyala@iiserb.ac.in, abhijit@iiserb.ac.in

Abstract

The principles of dynamic covalent chemistry (DCC) allow precise integration of molecular building units, resulting in highly crystalline framework structures, known as covalent organic frameworks (COFs). By employing the toolkits of DCC, the post-synthetic linker exchange (PLE) has emerged as an effective strategy for constructing highly crystalline COFs from various preassembled entities. Inspired by the exciting features of PLE, our group developed a straightforward approach to transform a porous organic cage into a highly porous, free-standing 2D COF membrane ($S_{\text{BET}} = \sim 1700 \text{ m}^2 \text{ g}^{-1}$) under ambient conditions at a faster timescale (24 h). The COF film showed high permeance and excellent molecular sieving performance. We have examined the initial stage dynamics of the above interfacial PLE process using pendant drop tensiometry elucidating the rapid COF growth. In this regard, COF fabrication at the liquid-liquid interface was simulated in tensiometric setup at optimized concentrations. The distinct early-stage interfacial behaviours of diverse synthetic routes (monomer-/cage-to-COF) were experimentally verified through mutually corroborative tensiometry, optical microscopy, electron microscopy, and PXRD analyses. Furthermore, the pivotal role of in situ generated imine intermediates (ImIs) and the phenomenon of spontaneous emulsification in accelerating the interfacial COF growth process was elucidated. The methodology developed to study the initial COF growth kinetics was also applied to a new interfacial PLE-mediated cage-to-COF transformation. The current study on deploying the pendant drop tensiometric technique to examine early-stage interfacial polymerization dynamics opens up a gripping avenue for mechanistic explorations in PLE-based COF synthesis.

18. FUNCTIONALIZED POLYMER NANOCOMPOSITES AS A PROMISING MATERIALS FOR INDUSTRIAL APPLICATIONS

Gautam Jaiswar

Department of Chemistry, Dr. Bhimrao Ambedkar University, Agra.
Email: gjaiswar@gmail.com

Abstract

Functionalization of polymers has recently become better understandable as a good tool to prepare composite materials possessing excellent thermal, mechanical, and other specific required

properties. Polymers are promising candidates to solve existing engineering problems, due to its low density and excellent mechanical performance. Large number of functional groups was successfully introduced in the past decades and there is still work is going on in this domain. Functional groups as like hydroxyl, epoxy, carboxylic or amino groups introduced into polymer backbone to achieve specific required properties in that polymer. In the present research work discussion were made on different properties of functionalized polymer nanocomposites materials by using different functional groups of poly(methyl methacrylate) (PMMA). Synthesis of amino functionalized PMMA using post polymer functionalization method by treating with four different amino compounds to obtain functionalized PMMA. Bonding behaviour of functionalized PMMA was characterized with Fourier transform infrared (FTIR) spectroscopy. Studies were highlighted on functionalized PMMA to prepare functionalized polymer nanocomposites by the addition of nanoclay and Ag nanoparticles into the polymer matrix. Behaviour of these nanocomposites were studied against thermal and antibacterial properties. Sophisticated analytical techniques i.e., thermal gravimetric analysis (TGA), differential thermal analysis (DTA) and derivative thermogravimetric curve (DTG) were reported to characterize the thermal properties of nanocomposites.

19. DFT AND ELECTRO-OPTICAL STUDY OF SOME FLC COMPOUNDS

Himangshu Roy, Asim Debnath, Debarghya Goswami and Sripada Haldar

Department of Physics, University of North Bengal, Siliguri, India 34013

Department of Physics, St. Joseph's College, Darjeeling, India 34104

Email: rs_himangshu@nbu.ac.in

Abstract

Ferroelectric liquid crystals (FLCs) that exhibit microsecond order switching has potential for display and other electro-optic applications. In this present work, the physicochemical properties of four biphenyl benzoate based ferroelectric liquid crystals, 3H3R, 4H2R, 4H5R, 5H3R, has been carried out by density functional theory (DFT) and electro-optical method. DFT study suggests that first FLC compound exhibits the shorter chain length while the last one has longer. Longer chain introduces higher flexibility but reduces spontaneous polarization and increases switching time (spontaneous polarization of 5H3R and 3H3R is 73 nC/cm^2 , 104.25 nC/cm^2 and switching time is $770 \mu\text{s}$, $410 \mu\text{s}$ respectively) Due to increased flexibility, longer chain molecules exhibits more number LC phases (5H3R, 4H5R) as compared to shorter chain molecules (4H2R, 3H3R). Higher dipole moment results in higher spontaneous polarization and faster switching time (dipole moment of 4H2R, 5H3R is 3.2728D, 3.1126D and spontaneous polarization 112.3 nC/cm^2 , 73 nC/cm^2 respectively). Phase transition temperature increases slightly due to strong intermolecular force stabilizing ferroelectric phase for the compound having large dipole moment like in the case of third and fourth compound (clearing temp 78°C and 79°C) Goldstone mode (GM) relaxation process was detected in ferroelectric SmC^* phase. But, as none of the compounds possessed SmA phase, no soft mode was observed, as reveal by dielectric spectroscopy measurement. High value of polarization, sub millisecond order switching time suggests potential use in display applications.

20. NANOCOMPOSITES OF SILVER DOPED TiO₂: SYNTHESIS, CHARACTERIZATION, AND APPLICATION

Himani Pachauri and Ashish Kumar

Agra College, Agra

Email: dolly10790@gmail.com

Abstract

Organic molecules derived from many sectors cause a variety of harmful contaminants in wastewater. This study is based on highlighting the synthesis of nanoparticles of doped TiO₂. The unique qualities of TiO₂-based photocatalysts, such as their nontoxicity, high capacity for photocatalytic destruction, and superior thermal and chemical stabilities, allow them to show exceptional absorption behaviour towards organic contaminants in wastewater. The most significant photocatalysts for use in environmental applications are thought to be nanosized TiO₂-based materials. Their advantages, like their reduced cost, higher activity, and chemical and photoresist qualities, are the reason they are being extensively researched. Ag-doped TiO₂ nanoparticles with anatase crystalline structure were synthesized by sol-gel process. Nanocomposites annealed at 500°C to form macry stalline structure of the anatase phase. Products morphological and optical properties were characterized by X-ray diffraction (XRD), energy dispersive X-ray microanalysis (EDS), UV-Vis diffuse reflectance spectroscopy (UV-VIS DRS), Field emission scanning electron microscopy (FE-SEM), and FTIR techniques. Scanning electron microscopy and transmission electron microscopy revealed the nano size of the products. This study explained the process of synthesis and characterization techniques of nanocomposites.

21. BIOMEDICAL MATHEMATICS: ADVANCES AND SOME CHALLENGES

J.C.Misra

Mathematics Department, IIT Kharagpur 21302

Email: misrajc@gmail.com

Abstract

In the beginning, discussion will be made of different disciplines of Biology and Medicine in which various mathematical methods have been applied by different researchers till now. This will be followed by a systematic discussion of different mathematical techniques used in mathematical modelling of different biomedical systems. Mechanical behaviour of the human arterial system (both arterial wall tissues and blood) will be of particular concern. Modelling of flow and heat transfer of blood will be explained as a particular example.

22. ATOM-ECONOMIC, HIGHLY EFFICIENT AND GREEN SYNTHESIS OF B-AMINOCARBONYL DERIVATIVES UNDER VISIBLE LIGHT RADIATIONS

Jaggi Lal and Asma Rani

Department of Chemistry, Sanskriti University, Mathura 81401, Uttar Pradesh, India

Email: jaggitajagra@gmail.com

Abstract

Despite various prior reports of effective catalytic and non-catalytic approaches towards the β -aminocarbonyl; a simple, efficient and green synthetic protocol for the synthesis of β -amino

carbonyl derivatives via Mannich reaction under visible light under solvent-free conditions has been described. No use of hazardous solvents in the protocol, hence making this process environment friendly. In view of green chemistry perspectives, various parameters including atom economy, atom-efficiency, carbon efficiency, reaction mass efficiency and optimum efficiency have been calculated and described for the newly developed procedure.

23. NEW TECHNIQUES FOR SIMULATING MASSIVE COLLECTIONS OF INTERACTING PARTICLES IN REALTIME

Jai Jayesh Bellare

Electrical Engineering, IIT Bombay, Powai, Mumbai – 400076

Email: 24b1307@iitb.ac.in

Abstract

New algorithms are developed for simulation of multiparticle interacting systems, on the order of 106 particles in real time. This is achieved by parallelizing the algorithm and using improved data structures more conducive for parallelization. This helps in simulating real-world systems. Equations describing these systems are straightforward. However, the naïve code implementation scales poorly [$O(n^2)$] with high particle counts, necessary to make the model behave realistically. This slowness makes it difficult to use; changing a single parameter requires recomputing the model for hours. These also require expensive professional-grade hardware to run on. The image/video rendering happens after the parameters are set, which makes it impossible to perturb the system interactively. Our new techniques run in real time on consumer-grade hardware, by fully utilising cache locality, vectorization, multithreading and GPUs. A model running 106 particles colliding at 60fps on an Intel i7 165G7 CPU and an NVIDIA MX330 GPU (moderate grade hardware), with interactivity, had speedup of many orders of magnitude compared to the single-threaded version. This was tested on an ideal gas model, and showed that the system follows the Maxwell-Boltzmann energy distribution. These new techniques have wide applications such as soft solids, membrane dynamics, cloth, fluids, and for solving differential equations on a grid, such as those modelling chemical reactions and phase changes. They can improve the daily workflow of a scientist trying to understand a system interactively, while also reducing the hardware required and power consumed.

24. POLYBENZIMIDAZOLE COMPOSITE MEMBRANES WITH SELF-CATALYTIC PROPERTIES: EFFECT OF REDUCED GRAPHENE OXIDE

Jay N. Mishra, Nitika Devi, Yong-Song Chen and Prabhakar Singh

Department of Physics, Indian Institute of Technology (BHU) Varanasi, Varanasi, India

Department of Mechanical Engineering and Advanced Institute of Manufacturing with High tech Innovations, National Chung Cheng University, Chiayi County 61301, Taiwan

Email: jaynarayanmishra.rs.phy20@itbhu.ac.in

Abstract

In this study, Polybenzimidazole (PBI)-based composite membranes were synthesized using Mn-doped titanium pyrophosphate (TMP) and graphite oxide (GO) prepared via the Hummers method. GO's oxygen functional groups not only significantly improved the dispersion of TMP

in the PBI matrix, as confirmed by FESEM and EDS, but also played a crucial role in imparting self-catalytic properties to the membrane. This key feature enhances its redox activity, providing a promising approach for fuel cell applications without the need for external catalysts. Thermal analysis showed stability up to 400°C, with a glass transition temperature (T_g) of 415°C and mechanical strength of 40 MPa. Electrochemical characterization in 1M Na_2SO_4 (pH = 7) further demonstrated the membrane's redox activity via cyclic voltammetry and linear sweep voltammetry, and Mott-Schottky analysis confirmed the membrane's bandgap nature. Fuel cell testing revealed improved performance, with PA-doped PBI/TMP membranes showing increased power densities from 314.0 to 395.2 mW cm^{-2} as the temperature rose from 150°C to 180°C, accompanied by reduced resistances. In conclusion, the self-catalytic behavior induced by GO, combined with the enhanced structural and electrochemical properties of the PBI/TMP/GO membrane, addresses a major challenge in fuel cell technology: cost reduction. By eliminating the need for expensive external catalysts, this self-catalytic membrane provides a cost-effective and efficient solution for high-temperature fuel cell applications.

25. NONLINEAR ABSORPTION OF HIGH INTENSITY LASER BEAM IN AN ARRAY OF CNT'S: FIELD PROFILE OPTIMIZATION

Kaisar Ali and Asheel Kumar

Plasma Physics Research Group, Department of Physics, University of Allahabad,

Prayagraj 11002, India

Email: kaisarali001@gmail.com

Abstract

The restoring force applied on the electron cylinder by the ion cylinder in the carbon nanotube after interaction with the highly intense linearly polarized Hermite cosh-Gaussian laser beam provide the oscillation of electron about ions. The electron starts collision with collisional frequency . The nonlinear absorption phenomena is observed. In this paper, we theoretically formulated the expression for the effective absorption coefficient of intense laser beam polarized along x-direction with propagating along y-direction and we observe that the effective absorption of laser beam profile in cylindrical shaped vertically aligned carbon nanotube achieved its peak value at resonance frequency $\omega=0.707\omega_{pe}$. The effective absorption coefficient is enhanced by tuning the parameters of laser beam profile e.g. normalized beam width (x / w_0), mode index (m), beam decentered parameter (d), normalized incident laser beam frequency (ω / ω_{pe}) as well as carbon nanotube parameters e.g. normalized radius (r_w / b), normalized collisional frequency (v / ω_{pe}). The absorption of laser beam in carbon nanotube has various application in biomedical, semiconductor electronics, sensors etc.

26. THE EFFECT OF WETT ABILITY ON THE GEL STRENGTH OF CAPILLARY SUSPENSION BY INSITU SURFACE MODIFICATION OF CUBE SHAPE HEMATITE PARTICLES.

Kalyani Kulkarni, Madhvi Tiwari and Venkateshwar Rao Dugyala

Department of chemical engineering, Indian Institute of Science Education and Research, Bhopal – 462066,

Madhya Pradesh India

Email: kulkarni23@iiserb.ac.in

Abstract

Capillary suspensions are three-phase systems with particles dispersed in a primary fluid and stabilized by a small amount of immiscible secondary fluid. While previous research has focused on isotropic particles, this study investigates the impact of wettability on the gel strength of capillary suspensions using anisotropic, cube-shaped hematite particles. These hydrophilic particles, dispersed in a water/glycerol mixture, form capillary bridges with oleic acid, the secondary fluid, which also acts as a hydrophobizing agent for in-situ surface modification. Rheological measurements show that increasing the secondary fluid concentration raises the gel strength due to the growing number of capillary bridges. However, beyond a certain point, further fluid addition leads to particle agglomeration, weakening the particle network and reducing yield stress. The study also examines a system where oleic acid is delivered with decane, revealing that a smaller amount of oleic acid produces a stronger increase in viscosity and yield stress compared to using pure oleic acid.

27. KINETIC AND ISOTHERM STUDIES FOR REMOVAL OF LEAD USING BENTONITE AND BENTONITE ACTIVATED CHARCOAL MIXTURE

Kumari Pallavi, Jha Ashok Kumar, Sharma Usha and Verma Sachin

Research Scholar, University Department of Chemistry, T.M. Bhagalpur University, Bhagalpur, Bihar, India.

Department of Chemistry, G.B. College Naugachia, T.M. Bhagalpur University, Bhagalpur, Bihar, India

Research Scholar, University Department of Chemistry, T.M. Bhagalpur University, Bhagalpur, Bihar, India

Email: ashokjha39@gmail.com

Abstract

The present study is aimed at devising a low cost and eco- friendly method of lead removal from aqueous medium. A comparative study of removal of Pb(II) by bentonite and bentonite activated charcoal mixture (I:I) was done. Batch experiments were done to find optimum condition as a function of variables such as pH, agitating time, initial concentration of Pb²⁺ adsorbent doses. The results showed that experimental results were the best fit for Langmuir isotherm. The kinetic studies confirmed the pseudo-first order reaction. The bentonite was characterised by TGA, DTA, XRD, and FITR. The maximum adsorption maximum adsorption capacity was evaluated to be 99.97percentage .Further uptake capacity by bentonite activated charcoal mixture was almost same as the bentonite. Bentonite activated charcoal mixture has emerged as a potential adsorbent of lead (II) ions from aqueous medium.

28. THE EFFECTIVE OF IONS IN CLOUD FORMATION, PRECIPITATION, AND THEIR INFLUENCE ON ATMOSPHERIC ELECTRICAL CONDUCTIVITY.

M. Chandra

Poornima Institute of Engineering and Technology, Jaipur

Email: mksh.rpt@gmail.com & mukesh.chandra@poornima.org

Abstract

The study of electrified clouds requires an understanding of the factors affecting their electrical conductivity. Researchers suggest that these clouds mainly have a positive dipole charge

distribution, impacting their electrical properties. Small ions in the clouds are influenced by cosmic ray ionization, leading to ion loss through various mechanisms. A major challenge in studying electrified clouds is the presence of electric fields that can disrupt ion conduction, making precise measurements of conductivity difficult, especially regarding small-scale space charge fields and individual charged particles. To address these challenges, researchers focus on charge transfer mechanisms in boundary regions and cloud updrafts, as well as the thickness of charge distribution in surrounding layers. This approach improves the understanding of electrified clouds' behavior and their conductivity. Thunderstorms with charged clouds and precipitation exhibit high electrical conductivity, which can vary due to different factors. However, relaxation time may not always be short, particularly in small-scale fields and individual particles, highlighting the need for further research into the complex dynamics of electrified clouds and their environmental effects.

29. PICKERING EMULSIONS: ROLE OF PARTICLE WETTABILITY AND ADHESIVE FORCE ON DROPLET BRIDGING

Madhvi Tiwari, M. G. Basavaraj and V. R. Dugyala

Soft and Active matter Research Laboratory (SAMRL), Department of Chemical Engineering, Indian Institute of Science Education and Research Bhopal, Bhopal, India - 462 066.

Polymer Engineering and Colloid Science Lab, Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, India - 600036.

Email: vdugyala@iiserb.ac.in

Abstract

This study demonstrates the engineering of Pickering emulsion gels by tuning particle positioning at the interface and adhesive forces. This is achieved through precise surface modification of hematite particles using oleic acid in a water-decane system. Microscopic observations revealed that these droplets are stabilized through bridging mechanism, where oil droplets are connected by sharing a monolayer of particles, with an intervening water layer between them. The role of particle position at interface and the adhesive force between particles and interface is examined as a function of oleic acid. The experimental observations reveal that, the concentration of oleic acid affects both the positioning of particles and adhesive forces, leading to the formation of partially covered droplets at specific oleic acid concentration ranges where the particle position and adhesive forces are favorable for the bridge formation. The versatility of the process is demonstrated by using different types of oil (dodecane, toluene, and chloroform) and modifiers (caprylic acid, myristic acid and stearic acid). In all the cases stable emulsions with partial coverages are obtained at precise concentration of the modifier. These emulsions show remarkable stability under undisturbed conditions due to gel like nature, however they can be destabilized by using external stimuli such as sonication or heating, therefore the reversibility, that is cyclic de-stabilization followed by stabilization of emulsions is examined. The proposed method results in re-stabilization of partially covered emulsions repeatedly. The effect of particle concentration and water to oil ratio on the bridged emulsions' stability and coverage is also studied.

30. EMPOWERING INDUSTRIAL WATER PURIFICATION THROUGH GREEN NANOTECHNOLOGY BY SUSTAINABLE BIO-NANOCOMPOSITE MEMBRANES FOR EFFICIENT DYE REMOVAL

Manas Mandal, Arathi, Roop Singh Lodhi and Paramita Das

Department of Chemical Engineering, Indian Institute of Science Education and Research Bhopal, M.P. 462066, India

Email: paramita@iiserb.ac.in

Abstract

The contamination of water by industrial effluents, particularly hazardous dyes, poses a serious threat to ecosystems and human health. Traditional remediation techniques such as chemical precipitation, coagulation, and activated carbon adsorption face challenges including secondary pollution, high costs, and limited efficiency. To address these issues, a novel bio-nanocomposite adsorptive membrane has been developed for the effective removal of dyes from wastewater. The membrane is fabricated using cellulose nanocrystals derived from rice straw (RSDCNCs), modified via dopamine oxidative self-polymerization, which enhances surface chemistry and adsorption capacity. The functionalized RSDCNCs are deposited onto Whatman filter paper using vacuum filtration, with poly(vinyl alcohol) (PVA) as a binder and glutaraldehyde as a crosslinker. The membrane's efficiency was tested using methylene blue (MB) dye, achieving over 95% removal efficiency. Optimal conditions included a pH range of 6.4–7, an initial MB concentration of 10 ppm, an adsorbent dosage of 0.04 g, and a shaking speed of 150 rpm. Under these conditions, the membrane reached a maximum removal efficiency of 98% after 4 hours. Adsorption kinetics followed a pseudo-second-order model, indicating chemisorption, and thermodynamic data fit the Langmuir isotherm, suggesting monolayer adsorption. Regeneration studies demonstrated that the membrane could be reused for up to five cycles with minimal performance loss.

31. SELF-PROPULSION DYNAMICS OF MAGNETIC ACTIVE PARTICLES UNDER MAGNETIC FIELDS

Megha Varma, Jatin Bhumarakar Snigdha Thakur and Venkateshwar Rao Dugyala

Department of Chemical Engineering, Indian Institute of Science Education and Research Bhopal, Bhopal, 462 066 Madhya Pradesh, India

Department of Physics, Indian Institute of Science Education and Research Bhopal, Bhopal, 462 066 Madhya Pradesh, India

Email: megha20@iiserb.ac.in

Abstract

Self-propulsion refers to the autonomous movement of micro, nano, or mesoscopic particles. In this study, anisotropic magnetic micro-swimmers (platinum-coated hematite@silica cube particles, HM@SiO₂ - Pt) with varying magnetic strengths were used to investigate their self-propulsion behaviour under the geomagnetic field, using hydrogen peroxide as a fuel. The particles exhibited different propulsion trajectories based on their magnetic strength, random motion resulting due to particle rotational diffusivity (D_R), and directed motion due to particle critical magnetic frequency (ω_c). The ratio of rotational diffusion time (τ_R) to magnetic relaxation time (τ_M) influences the trajectories: $\tau_R/\tau_M \gg 1$ leads to straight paths, $\tau_R/\tau_M \ll 1$ results in random motion over extended periods, and $\tau_R/\tau_M \approx 1$ produces meandering-like paths. The magnetic

field's impact on particle motion was further quantified by simulating trajectories at different ω_c values, with experimental and simulated results aligning. Additionally, experiments demonstrated the ability to control particle trajectories to form complex patterns under an external magnetic field.

32. GREEN SYNTHESIS OF CO & NI CO-DOPED CUO NANOPARTICLES AND THEIR MORPHOLOGICAL AND BIOLOGICAL ACTIVITIES

Neelam and Devendra Kumar

Department of Chemistry, Institute of Basic Sciences,

Dr. Bhimrao Ambedkar University, Khandari Campus, Agra 82002

E.mail: devendrakumar131@gmail.com

Abstract

In the present study green sustainable, simple and cost effective synthesis and determination of the antibacterial and antifungal activity of pure, doped and Co and Ni codoped CuO NPs have been reported. The FTIR spectra of all synthesized NPs showed bands in the metal sensitive region may be attributed due to M–O bond indicating the formation of metal oxide nanoparticles. The size and morphology of the nanoparticles were determined by P-XRD and FE-SEM studies respectively. Energy-dispersive X-ray analysis was used to determine the elemental composition of the nanoparticles. P-XRD results revealed that the particle size of synthesized nanoparticles exist in the nanometer range. The morphology of the pure CuO has been changed after codoping with Co and Ni as indicated by FE-SEM. The synthesized nanoparticles were screened for antibacterial activity *in vitro* against two gram negative bacteria *Klebsiella pneumoniae* and *Pseudomonas aeruginosa* while antifungal activity against *Candida albicans* by adopting disk diffusion method. The results of antibacterial and antifungal studies exhibited potential antimicrobial activity. These investigations could be used in antibiotic development which further gives a direction for biomedical applications.

33. A STUDY ON PHYTOCHEMICALS: SYNTHESIS AND ITS APPLICATIONS

Nikhat Fatima, Arzoo Siddiqui, Amulya Sinha, Girish Singh, Amit Yadav and Sharda Sundaram Sanjay

Department of Chemistry, Ewing Christian College, University of Allahabad, Prayagraj, Uttar Pradesh, India 11003.

Email: sharda100@rediffmail.com

Abstract

Phytochemicals are biologically active chemical compounds including carotenoids, flavonoids, terpenes, polyphenols, etc., naturally found in plants and possess a wide spectrum of biological activities include antioxidant and antimicrobial activities, detoxification enzyme modulation, and immune system stimulation, as well as hormone metabolism modulation with multifaceted uses. They deliver medical services for humans beyond those attributed to normal nutrients. Phytochemicals are not nutritious, and they are not needed by the human body to sustain life, but they do have important properties to prevent or resist some common diseases. Therefore, the phytochemicals can be used in various perspectives that are associated with decreasing the chances of cancer, DNA genotoxic stress, and specific chronic diseases like cardiovascular disease, hypertension and obesity. Phytochemicals can be obtained from various sources including the agri-food products, leaves of various plants and from certain edible flowers like

silk cotton tree and dog flower. Phytochemicals are non-nutritive components of plants that are synthesized through biosynthetic pathways involving enzymatic reactions. Phytochemicals can be extracted from plant parts like leaves using a solvent, then concentrated and purified using chromatographic techniques. The isolated compounds can then be analyzed using spectroscopic techniques and chemical methods. Several studies over the past decade have shown promising applications of phytochemicals in drug delivery and treatment. Therefore, we observe a rising trend of applications of phytochemicals in clinical science. Recent scientific studies have also shown the promising application of phytochemical compounds as nanoparticles in cancer research, cosmetics, and food supplements.

34. SOIL ORGANIC MATTER RESEARCH AND CLIMATE CHANGE: MERELY RESTORING CARBON VERSUS RESTORING SOIL FUNCTIONS

Pancham Kumar and Ravi Prakash

Department of Chemistry, BSA College, DR BR Ambedkar University Agra

Email: beingsachinsir@gmail.com

Abstract

Over the last two decades, the sequestration of carbon in soils has often been advocated as a solution to mitigate the steady increase in the concentration of CO₂ in the atmosphere, one of the most commonly mentioned causes of climate change. A large body of literature, as well as sustained efforts to attract funding for the research on soil organic matter, have focused on the soil carbon sequestration – climate change nexus. However, because CO₂ is not the only greenhouse gas released by soils, and given the fact that the feasibility of large-scale carbon sequestration in soils remains controversial, this approach does not appear optimal to convince policy makers to invest in soils. In this perspective article, we argue that a far better strategy revolves around the effect of climate change on functions/services that soils render. In particular, since climatologists forecast less frequent but more intense rainfall events in the future, which may lead to food shortages, catastrophic flooding, and soil erosion if soils are not able to cope, a more suitable focus of the research would be to increase soil organic matter content so as to strengthen the water regulation function of soils. The different conceptual and methodological shifts that this new focus will require are discussed in detail.

35. ADVANCED FUNCTIONAL MATERIALS FOR MULTIFUNCTIONAL APPLICATIONS

Parasharam M. Shirage

Department of Metallurgical Engineering and Materials Science,

Indian Institute of Technology Indore-453552. INDIA.

Email: pmshirage@iiti.ac.in , paras.shirage@gmail.com

Abstract

The recent advancement in advanced functional materials for energy generation, storage and sensors are of great potential. In this talk recent advancement in materials for battery,

supercapacitor and sensors will be reviewed and presented. The optimization of processing parameters in the growth of these materials will be reviewed. The results obtained by Physico chemical characterization and their influences on battery performance will be discussed. The effect of processing parameters on Na-ion batteries and sensors will be discussed in detail. The emerging materials related to Sodium Ion Battery applications will be discussed. Sodium-ion batteries (SIB) are emerging as an alternative energy storage device to Lithium Ion Batteries (LIB). Literature on the cathode and anode materials, battery fabrication, and testing results will also be presented.

36. SYNTHESIS OF BIMETALLIC BIVALENT METAL COMPLEXES OF SCHIFF BASE DERIVATIVE FROM DIACETYLMONOOXIME AND P-PHENYLENEDIAMINE

Ravi Prakash, Ritu Rani Chaudhary and R.B. Singh

Department of Chemistry, B.S.A. College, Mathura 81004, U.P. (India)

Department of Zoology, School of Life Sciences, Dr. Bhimrao Ambedkar University, Khandari Campus, Agra – 282002 (U.P.) India

Email: drravichem@gmail.com; ritumjp@gmail.com; rbsinghugc@gmail.com

Abstract

The Schiff bases and their metal complexes derived from -diketones and -ketomonooxime have wide industrial and biological applications. The coordination complexes of Schiff bases have been studied extensively due to their potential donor ability and strong complexing properties. In present work we report the preparation and characterization of some bivalent metal complexes of bis- diacetylmonooxime-p-phenylenediamine (BDMPDH₂). The bimetallic complexes of Mn (II), Co (II), Ni (II), Cu (II), Zn (II), Cd (II) and Hg (II) with Schiff base of p-phenylenediaminewith diacetylmonooxime (BDMPDH₂) composition M₂(BDMPD)₂(H₂O)_n (n=4 for, Mn²⁺, Co²⁺, Ni²⁺ or Cu²⁺ and n=zero for Zn²⁺, Cd²⁺ or Hg₂) and M₂(BDMPDH₂)Cl₄ have been prepared and characterised from magnetic susceptibility measurement and studies of IR and electronic spectra of complexes.

37. CHARACTERISTICS OF TEXTILE WASTE WATER OF SANGANER (RAJASTHAN) AND ITS PHOTOCATALYTIC DEGRADATION WITH ZNO CATALYST

Rekha Rani Agarwal and Mugdha Gupta

Chemistry Department, Poornima Institute of Engineering and Technology, Jaipur

Dr. Sampurnanand, Government Medical College, Jodhpur, Rajasthan

Email: drrragarwal@gmail.com

Abstract

During the last decade, Sanganer has developed into a leading place in the textile industry in India. The water used in textile industry is almost entirely discharged as waste. The effluents are very complex, containing salt, surfactants, ionic metals and their metal complexes, toxic

organic chemicals, biocides, and toxic anions, which are harmful to both flora and fauna existing on our planet. Degradation of these non-biodegradable organic compounds is not possible by conventional treatment processes. The analysis of waste water with different quality parameters and photocatalytic bleaching was examined by using UV light in photochemical reactor with ZnO catalyst.

38. DESIGN AND ANALYSIS OF HIGH-FREQUENCY T-SHAPED MICROSTRIP PATCH ANTENNA

Renu Sharma and Mansi Arora

Department of Physics, JECRC UNIVERSITY, Jaipur

Central Electronics Engineering Research Institute (CSIR), Pilani, India

Email: renu.malsaria@gmail.com

Abstract

In this paper, a T-shaped microstrip patch antenna is designed and analyzed using HFSS software for operation at millimeter-wave frequencies. A circular cut is introduced at the bottom of the patch to enhance the antenna's performance, improving efficiency. The antenna design uses Rogers RT/Duroid 5880, Dielectric loss tangent 0.0009, and Dielectric constant 2.2 as the dielectric substrate, known for its low dielectric constant and low loss, making it suitable for high-frequency applications. The overall size of the proposed antenna is $2.59 \times 1.38 \times 1.38$ mm³; the feeding technique uses a 50Ω feed line to the antenna. The performance parameters such as return loss, Voltage Standing Wave Ratio (VSWR), gain, directivity, and bandwidth are evaluated at 38 GHz frequency. Introducing a slot with a rectangular T-shaped patch antenna achieved a higher frequency optimized radiation efficiency and gain of the proposed antenna at 6.16 dB. The fractional bandwidth is 10.79 % with a VSWR of 5.9945 and return loss at 3.022 dB. which is essential for 5G communication systems and other high-frequency applications.

39. NUMERICAL SIMULATION AND INVESTIGATION OF MoS_2 BASED HETEROJUNCTION SOLAR CELLS

Ritishri Priyaranjan Pradhan and Arvind Kumar

Department of Physics, University of Allahabad, Prayagraj 11002, India

Email: ritishrajp@gmail.com

Abstract

Sustainable green clean energy sources centered solar energy to electrical energy conversion is a predominate requirement for developed society. A solar cell or photovoltaic cell acts as a major part of that to fulfill the energy interest. Two-dimensional materials such as MoS_2 -based heterojunction solar cells attracted researchers for their extraordinary chemical, physical, thermal, mechanical, optical, and electrical stability. In this work, we simulated the electrical behavior of n- MoS_2 /p-Si-based heterojunction-based solar cells with the help of SCAPS D simulation tool. We evaluated the performance of MoS_2 -based solar cells by varying the active layer's thickness, which leads to the changing of the band gap, variation in the electron affinity, and change in

interfacial defect, and by varying the working temperature of the devices. The best combinations of different parameters give an efficiency of 12%, which is sufficiently high enough as compared to what was reported, previously. This will provide basic insight into the development of high-performance solar cells with 2D materials.

40. GREEN DEVELOPMENT TECHNIQUES: GREEN CHEMISTRY

Rudraksh Srivastava and Amulya Sinha

Department of Chemistry, University of Allahabad, Prayagraj, Uttar Pradesh, India.

Department of Chemistry, Ewing Christian College, University of Allahabad, Prayagraj, Uttar Pradesh, India.

Email: rudrakshsrivastavachemistry@gmail.com

Abstract

Green chemistry is all about making chemistry safer and more sustainable for our planet. This presentation will explore exciting ways to make chemical processes cleaner and more efficient. At its core, green chemistry focuses on reducing waste, using safer materials, and finding energy-efficient methods.

One major development is the use of eco-friendly catalysts, which help speed up chemical reactions without needing extreme conditions. This not only saves energy but also reduces harmful by-products. Another promising area is biocatalysts, where we use natural enzymes and microorganisms to create important products like medicines in a much greener way.

We'll also look at methods that avoid harmful solvents, such as solvent-free reactions and those done in water, which are better for the environment. Techniques like microwave-assisted synthesis and flow chemistry are making reactions faster and cleaner, leading to less waste overall.

Additionally, using life cycle assessments (LCA) helps us understand the environmental impact of different chemical processes, allowing us to choose the most sustainable options. By focusing on recycling and reducing waste, green chemistry promotes a circular economy.

Through real-life examples and emerging trends, this talk will show how green chemistry is paving the way for a more sustainable chemical industry. Join us to discover how these innovations can help protect our environment while supporting progress in science and technology.

41. PHYTOREMEDIATION POTENTIAL OF BRASSICA JUNCEA L. GROWN IN DIFFERENT CD AND PB POLLUTED SEWAGE IRRIGATED SOILS

Rupesh Kumar Ojha, Dinesh Mani, Devi Prasad Shukla, Himanchal Vishwakarma, Jeetendra Verma, Manoj Kumar and Suraj Patel

Sheila Dhar Institute of Soil Science, Department of Chemistry, University of Allahabad, Prayagraj, Uttar Pradesh, India, 211002

Email: ojharupeshkumar5@gmail.com*

Abstract

The current research work is mainly focused on the evaluation of the phytoremediation potential of *Brassica juncea* L. grown in different sewage irrigated sites in Prayagraj, Uttar Pradesh. The representative soil and plant samples were collected from different sewage irrigated sites in Prayagraj viz., Naini, Preetam Nagar, Daraganj and Rajapur. The heavy metals Analyzed plant samples were showed the various concentrations of Cd and Pb ranged from 3.51 ± 0.16 $.97 \pm 0.09$,

3.69±0.25 .25±0.12 and 4.78±0.20 .11±0.17, 5.13±0.23 .06±0.21 mg kg in the roots and shoots respectively. The found results were showed that the maximum accumulation of Pb 5.13 followed by Cd 3.69 mg kg was recorded in the plant shoots at Naini sewage irrigated site. Maximum roots, shoots dry biomass yield was found at Rajapur sewage irrigated site polluted with Cd and Pb ranged from 3.10±0.07, 12.10±0.51 and 3.77±0.11, 12.81±0.32 g plant, respectively. Whereas minimum roots, shoots dry biomass yield i.e., 1.56±0.03, 10.05±0.32 and 2.09±0.04, 10.48±0.27 g plant was observed from Cd and Pb polluted soils at Naini sewage irrigated site, respectively. The values of BAF and TF of all Cd polluted soil ranged from 1.063±0.08 .300±0.06 and 1.051±0.10 .142±0.04 mg kg, respectively. Whereas the values of BAF and TF of all Pb polluted soils ranged from 1.075±0.11-0.987±0.03 and 1.073±0.13-0.983±0.07 mg kg, respectively. Almost all the values of BAF and TF >1 that proved *Brassica juncea* L. was a hyperaccumulator plant. Thus, *Brassica juncea* L. has greater importance in phytoremediation of heavy metal contaminated soils.

42. EXTRA-ORDINARY TRANSMISSION: FROM SUB-WAVELENGTH PLASMONIC APERTURES TO APERTURELESS METAGRATINGS

Sachin Kumar Srivastava

Department of Physics, Indian Institute of Technology Roorkee, India

Center for Photonics and Quantum Communication Technology, Indian Institute of Technology Roorkee, India

Email: sachin.srivastava@ph.iitr.ac.in

Abstract

In 1944, Hans A. Bethe predicted theoretically that transmission efficiency of light passing through any aperture is given by the following equation [Bethe, Phys. Rev. **66**, 163 (1944)],

$$\text{Transmission Efficiency} = \frac{64}{27\pi^2} (kr)^4 \sim \left(\frac{r}{\lambda}\right)^4 \quad (1)$$

where, $k = 2\pi/\lambda$ is

propagation constant of the incident light of wavelength λ and r is the width of the aperture. For sub-wavelength apertures $r \ll \lambda$, according to equation (1), the transmission efficiency is close to zero. However, in 1998, Ebbesen et.al. experimentally demonstrated about 6% transmission through subwavelength nano-holes of silver [Ebbesen et al., Nature **391**, 667 (1998)]. This transmission was attributed to the funnelling of light through the excitation of surface plasmons and was named as extra-ordinary optical transmission (EOT). Nanostructured plasmonic configurations possess resonant optical excitation of surface electromagnetic waves (SEWs) under suitable optical excitation. These resonant phenomena lead to enhanced electromagnetic fields by several orders of magnitude, thereby leading to intriguing vast range of applications. The excitation of surface plasmons leads to conversion of light to SEWs of sub-wavelength attributes, which are beyond diffraction limit. EOT through a meta-grating comprising of two metal nano-slit arrays (MNSAs), where the opening of one MNSA is blocked by the closed portion of the other MNSA and vice versa will be discussed. An EOT through an opening of $\lambda/65$ with more than 90% transmission efficiency was achieved. The role of plasmonic coupling resulting in giant EOT was assessed and experimentally confirmed in an *apertureless* plasmonic metagrating. Such metagratings find applications in polarizers, frequency selective surfaces, sensors, etc.

43. BENZOXAZOL COMPOUND SAND THEIR COMPLEXES SYNTHESIS AND MESONIC CHARACTERIZATION

Sanjeev Kumar Gupta, Abhay Pratap Singh and M. Karunakar

Department of Chemistry, Ewing Christian College, Prayagraj 211003, India

Email: sanjeev50100@gmail.com

Abstract

Liquid crystal material 5-(alkoxy) -(((4-(5-methylbenzoxazol -yl)- phenyl)imino)methyl)phenol, HLn (n = 10, 12, 14) and their copper(II) complexes had been synthesized; molecular structures of all the organic compounds and the metal complexes were elucidated by various spectroscopic techniques along with elemental analyses. Thermotropic properties were investigated by a combination of POM observation, DSC analysis and Xray diffraction experiments. All members of the series exhibit enantiotropicsmectic-A (SmA) mesophase. DFT calculations imply stable electronic structure of the ligand; HLn (n = 12) as well as of its copper(II) complex. Alkoxy-derivatives of methyl substituted benzoxazolemesogens, HLn series, were synthesized. All the compounds were found to be mesogenic, characteristic of enantiotropicSmA phase. Upon coordination to copper(II) metal ion, the resulting square planar copper (II) complexes of all the ligands retained SmA mesophase while their isotropic temperatures were found to be higher.

44. DISSOLUTION-INDUCED NATURAL CONVECTION: A STEFAN PROBLEM

Satyajit Pramanik, Subhankar Nandi, and Jiten C. Kalita

Department of Mathematics, Indian Institute of Technology Guwahati, Guwahati- 781039 Assam, India

Email: satyajitp@iitg.ac.in

Abstract

The classical Stefan problem, that is observable in melting, evaporation of droplets, freezing, casting, etc., aims to model the boundary evolution caused by the heat diffusion between the phases of a stationary material. Researcher have extensively studied these problems using analytical and numerical methods, and more recently there is a growing interest in problems involving the moving phase-change materials which have some externally provided motion. In this study, we investigate dissolution of solute in a solvent placed in a horizontal concentric cylinder. Theoretical investigation solves a Stefan problem with phase transition due to natural convective flow. To realize the objective, the governing equation for the concentration distribution, stream function–vorticity form of the Navier-Stokes equation for the flow field, and a Stefan condition for calculating the timescale evolution of the front are coupled together with different parameters. These non-linear equations are solved using a stable and second-order accurate boundary-fitted alternating direction implicit scheme with third-order QUICK upwind difference approximation for convective terms. The numerical scheme is validated initially by applying it to solve a natural convection problem with no phase transition, for which benchmark solutions are available. The validated scheme is then applied to the chosen problem followed by a refinement study to obtain a reliable solution. The obtained results are used to analyse the effect of physical parameters such as the Stefan number, geometric aspect ratio of solute to fluid, the Rayleigh number and the Schmidt number on dissolution rates as well as the flow patterns.

45. SYNERGISTIC EFFECTS OF WO_3 NANOPARTICLES AND $\text{Ti}_3\text{C}_2\text{T}_x$ MXENE FOR EFFICIENT ETHANOL GAS SENSING

Satyam Tripathi and Pratima Chauhan

Centre of Material Sciences, University of Allahabad, Prayagraj, India- 211002

Advanced Nanomaterials Research Laboratory, U.G.C. Centre of Advanced Studies, Department of Physics, University of Allahabad, Prayagraj, India- 211002

Email: satyam.phd2022@allduniv.ac.in

mangu167@yahoo.co.in

Abstract

In this research, we developed a novel sensing sensor based on a $\text{WO}_3/\text{Ti}_3\text{C}_2\text{T}_x$ nanocomposite for detecting ethanol gas at ppm levels at room temperature. The nanocomposite, which includes WO_3 nanoparticles and two-dimensional $\text{Ti}_3\text{C}_2\text{T}_x$ (MXene), was synthesized using an ultrasonic method. We conducted comprehensive morphological and structural analysis using techniques such as field emission scanning electron microscopy, X-ray diffraction, and nitrogen adsorption-desorption. The gas sensing performance of the $\text{WO}_3/\text{Ti}_3\text{C}_2\text{T}_x$ nanocomposite sensors was evaluated by measuring their response and selectivity to various target gases at room temperature. The sensors demonstrated a significant response to ethanol concentrations ranging from 25 to 300 ppm. Notably, the sensor achieved a high response value of 21.8 for 300 ppm ethanol, additionally; the sensor exhibited a rapid response time of 30 seconds and a recovery time of 42 seconds. The enhanced sensing capabilities are attributed to the synergistic effects between the WO_3 nanoparticles and the layered structure of the 2D $\text{Ti}_3\text{C}_2\text{T}_x$. This combination provides a large number of gas adsorption sites and an efficient conductive pathway, facilitating effective charge transport. These findings highlight the potential of the $\text{WO}_3/\text{Ti}_3\text{C}_2\text{T}_x$ nanocomposite as a highly sensitive and selective material for ethanol gas detection at room temperature.

46. NOVEL IMAGE ENCRYPTION SCHEME USING MODIFIED LOGISTIC MAPS BASED ON PRIMITIVE POLYNOMIALS

Shalini Gupta, Kritika Gupta and Nitish Thakur

Department of Mathematics & Statistics,

Himachal Pradesh University, Shimla 71005

Email: shalini.garga1970@gmail.com, kritika993@gmail.com, nitishthakur151@gmail.com

Abstract

In this paper, we present a novel approach to image encryption utilizing a modified logistic map integrated with a primitive polynomial over \mathbb{Z}_m . Chaotic maps are well known for their sensitivity to initial conditions and parameters, properties that are crucial for secure cryptographic systems. However, traditional chaotic maps like the logistic map suffer from limitations when applied directly in discrete systems or constrained environments. To address this, we modify the logistic map by introducing a transformation governed by a primitive polynomial over \mathbb{Z}_m . This modification enhances the chaotic properties, allowing for stronger diffusion and confusion across the pixel values of an image. The chaotic sequence generated is used to permute and mask pixel values, creating a highly secure and randomized encrypted image. We perform extensive testing of the chaotic properties of the proposed map, including Lyapunov exponent calculations, bifurcation

analysis, and sensitivity to initial conditions, confirming its suitability for cryptographic applications. Further, we rigorously test the proposed scheme for key sensitivity, randomness, and statistical properties using a variety of metrics, including histogram analysis, correlation coefficients, and entropy calculations. Additionally, we perform cryptanalytic assessments to evaluate the scheme's resistance to common attacks, such as brute force and differential attacks. The results demonstrate that the modified chaotic map significantly enhances security while maintaining computational efficiency, making it practical for real-time image encryption in resource-constrained environments.

47. ELECTROCHEMICAL BIOSENSORS FOR SERUM BASED CANCER BIOMARKER DETECTION

Shilpa N. Sawant

Chemistry Division, Bhabha Atomic Research Centre, Trombay, Mumbai-400085

Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India.

Email: stawde@barc.gov.in

Abstract

Cancer is one of the major health challenges worldwide. Its detection in the early stage is crucial for an effective treatment. One of the conventional technique for detection of cancer is based on estimation of cancer biomarkers, which are basically biological molecules found in blood, other body fluids, or tissues that is a sign of a normal or abnormal condition or disease. Electrochemical biosensors offer a promising platform for development of sensors for detection of cancer biomarkers. As some of the cancer biomarkers often lack specificity and sensitivity, simultaneous detection of multiple biomarkers can make the diagnosis more accurate. To address this, mediator and substrate-free amperometric biosensor has been developed for simultaneous detection of cancer biomarkers carcinoembryonic antigen (CEA) and alpha-fetoprotein (AFP) by designing two different redox-labelled detection probes. In another work, carbon dots were synthesized by the hydrothermal method and bioconjugated with an antibody to design a nanoprobe for the detection of prostate specific antigen (PSA), an important serum based prostate cancer biomarker. The detection probe enabled biomodal assay of PSA via fluorescence and electrochemical sandwich immunoassay.

48. MICROWAVE ASSISTED SYNTHESIS OF MOLYBDENUM DOPED TiO₂ NANOCOMPOSITES VIA SOL-GEL METHOD

Shivalini Singh and Ashish Kumar

Department of Chemistry, Agra College, Agra

Email: ashishx1@rediffmail.com and shivalini.chaharag@gmail.com

Abstract

Microwave assisted sol-gel synthesis was utilized to create the Mo-doped TiO₂ nanoparticles. Using 2-propanol and titanium tetra isopropoxide as precursor materials, we obtained the results of this study, which were then calcined at 650°C to form the rutile phase. Transmission electron microscopy (TEM), field emission scanning electron microscopy (FE-SEM) were utilized to characterize the crystalline structure, chemical valence states, and morphology of

TiO₂ nanoparticles, and X-ray diffraction (XRD) was employed to characterize the as-prepared samples. The TiO₂ nanoparticles' rutile phase has formed, as shown by the XRD data. When TiO₂ nanoparticles were doped with 2% Mo, their band gap energy was 2.56 eV less than that of TiO₂. The size of the Mo-doped TiO₂ crystallite is likewise observed to be significantly smaller than that of the undoped TiO₂ crystallite. Because of their high specific surface area and low band gap energy values, the synthesized semiconductors would be very beneficial in photocatalytic applications.

49. ROLE OF GREEN SYNTHESIZED METALLIC/METALLIC OXIDE NANOPARTICLES IN COMBATING PHYTOPATHOGENS

Shivangi Sharma, Vishwajeet Singh, Akhilesh Kumar, Sanjay Kumar Kataria, Rajneesh K. Agnihotri and Gautam Jaiswar

Department of Chemistry, Dr. Bhimrao Ambedkar University, Agra

Department of Botany, BSA (PG) College, (Dr. Bhimrao Ambedkar University, Agra), Mathura

Department of Botany, Dhanauri PG College, Dhanauri, Haridwar

Department of Botany, Dayalbagh Educational Institute (Deemed to be University), Agra

Department of Botany, Dr. Bhimrao Ambedkar University, Agra

Email: shivangisharmabarhan@gmail.com

Abstract

Phytopathogens such as fungi, bacteria, and viruses drastically affect global agricultural productivity and enhance food scarcity by causing catastrophic diseases in several crops worldwide. However, the current system to combat phytopathogens heavily relies on the extreme use of chemical pesticides, which not only boost the agricultural economy and meet global food demand but also severely deteriorate human health and the environment. So, metallic nanoparticles have emerged as accountable materials that have caught the interest of plant pathologists due to their tremendous physicochemical properties. Moreover, the conventional methods for nanoparticle formulations use toxic, non-biodegradable, and expensive chemical agents. In contrast to traditionally synthesized nanoparticles, green nanoparticles fabricated through plants, biomolecules, and microbes are cost-effective, biodegradable, non-hazardous, have been proven to be more promising bioagents against phytopathogens, and provide an alternative eco-friendly approach for the control of phytodiseases. Therefore, the employment of nanoparticles fabricated through green methods promotes the sustainable development of farming systems across the world. The goal of this review is to demonstrate the drawbacks of the available traditional methods for nanoparticle fabrication and provide an overview of the various existing green strategies for nanoparticle fabrication, their advantages, and their effective role in the control of phytopathogens.

50. HUMAN WASTE MANAGEMENT IN THE SUB-ZERO TEMPERATURE

Shiwangi Dogra, Balendu Shekhar Giri, Dhananjay Singh and Manish Kumar

School of Engineering, University of Petroleum & Energy Studies, Dehradun, Uttarakhand 248007, India

Department of Chemical Engineering, IET, Lucknow, Uttar Pradesh, 226021, India

Escuela de Ingeniería y Ciencias, Tecnológico de Monterrey, Campus Monterrey, Eugenio Garza Sada 2501 Sur, Monterrey, 64849, Mexico

Email: balendus.giri@ddn.upes.ac.in; balendushekher23@gmail.com

Abstract

Human activities generate a diverse range of waste, but our specific focus is on human fecal waste, which presents a significant environmental challenge. This issue is particularly pressing in colder climatic regions with harsh conditions, complicating waste management. To address this, anaerobic septic tanks employing microbial degradation are the primary method. However, the reduction in microbial activity in cold temperatures poses challenges, leading to the slow degradation of human waste, especially in mountainous trails with dense populations. This paper thoroughly explores available energy-efficient technologies applicable in the Himalayan terrain to overcome these challenges. The primary objective is to identify alternative approaches for managing human waste in the Himalayan region. Research highlights significant challenges associated with anaerobic digestion, necessitating advancements in implementation.

51. RECENT ADVANCES AND FUTURE PROSPECTS OF QUANTUM BIOLOGY

Shri Niwash Singh

Department of Chemistry, H.D. Jain College, V.K.S. University, Arrah

Email: snsingh1214@gmail.com

Abstract

Quantum biology is the field of study of applications of quantum mechanics and theoretical chemistry to biological systems and processes at the atomic, molecular and organismal levels. It is an interdisciplinary field connecting quantum physics, biophysics, chemistry, biochemistry, biology and medicine. E. Schrodinger's book 'What is Life?' describes applications of quantum mechanics in biology. Living systems are fundamentally quantum mechanical in nature since the dynamics of their molecular, atomic and subatomic chemical systems are governed by laws of quantum physics. Recently developments in experimental techniques such as single-molecule spectroscopy, ultra-fast spectroscopy, time-resolved spectroscopy and other tools have enabled to study biological dynamics on increasingly small length and time scale for the processes necessary to the function of the living systems. A number of specific mechanisms within living cells that make use of the non-trivial characteristics of quantum mechanics such as quantum tunneling, quantum coherence, superposition and quantum entanglement, were not thought to be relevant to the mechanisms responsible for life to molecular, atomic and subatomic systems. The present review provides an outline of the current status and future prospects of quantum biology. Furthermore, phenomena such as photosynthesis, enzyme catalysis, olfaction and magnetic reception has also been explained more speculative for biomedical and emerging disease prevention.

52. ENHANCED RGO/WO₃ NANOHYBRID FILMS FOR ROOM-TEMPERATURE NO₂ DETECTION

Shubham Tripathi and Prem Prakash Singh

Ewing Christian College, Prayagraj, Uttar Pradesh, India 11003

Email: shubhamtripathi1708@gmail.com

Abstract

A room-temperature operable NO₂ gas sensor was developed hydrothermal method, resulting in tungsten oxide and reduced graphene oxide (rGO/WO₃) nanocomposite films. The microstructure

and morphology of these films were analyzed using X-ray Photoelectron Spectroscopy (XPS), X-ray diffractometer (XRD), Scanning Electron Microscopy (SEM), and Transmission Electron Microscopy (TEM). Detailed measurements of the electrical and NO₂ gas-sensing properties of WO₃ with varying amounts of rGO were conducted at room temperature to understand the role of rGO in enhancing NO₂ gas detection. The NO₂ gas-sensing mechanism of the rGO/WO₃ nanocomposite films was elucidated based on their composition and microstructures. The rGO/WO₃ nanocomposite film-based sensor demonstrated a strong response to low NO₂ gas concentrations at room temperature, with satisfactory linearity and long-term stability.

53. PARAMETRIC DECAY OF HIGH POWER LASER IN NANOCLUSTER PLASMA WITH EXTERNAL MAGNETIC FIELD

Sujeet Kumar and **Asheel Kumar**

Plasma Physics Research Group, Department of Physics, University of Allahabad, Prayagraj, India

Email: stkr0512@gmail.com

Abstract

In this theoretical study, we explore the parametric decay of a skew cosh-Gaussian laser into two electromagnetic waves and, within a collisional magnetized plasma embedded with spherical shaped nanocluster by considering a rippled density Langmuir wave pre-existed in the plasma. The external magnetic field is oriented perpendicular to the electric field of the skew cosh-Gaussian laser. The interaction of high power electric field of skew cosh-Gaussian laser with the clouds of nanoclusters might have potential to exert a ponderomotive force to the plasma electrons and rapidly transforms the nanoclusters into plasma balls, inducing oscillatory velocity to the electron cloud aligned with the electric field of the laser beam. The typical laser intensity is of the order of 10^{15} W/cm. The parametric decay is enhanced due to applied ambient magnetic field and strongly depends on nanocluster plasmon resonance and the phase matching conditions introduced through a rippled density plasma. The resonance condition is achieved at which the growth rate is maximum. Furthermore, it is found that growth rate get strengthened on increasing the skewness parameter and order of the skew ChG laser beam.

54. ENHANCEMENT IN DOWN-SHIFTING, UPCONVERSION, AND QUANTUM CUTTING EMISSION BY MULTIPLE TIMES HEATING OF TB³⁺/YB³⁺ DOPED LANBO₄ PHOSPHOR AND ITS APPLICATION AS GREEN LED SOURCE, ANTI-COUNTERFEITING, AND SOLAR CELLS.

Sumit Modanwal, **Abhishek Roy**, **H. Mishra** and **S. B. Rai**

Department of Physics, Institute of Science, Banaras Hindu University, India 221005

Department of Physics, Faculty of Science, University of Allahabad, India 211002

Email: sumitmodanwal375@gmail.com, sbrai49@yahoo.co.in, hmishra@bhu.ac.in

Abstract

The rare-earth-doped phosphor materials have wide applications in optoelectronic devices such as Light-emitting Diodes, Anti-counterfeiting, Bio-sensors, optical sensors solar cells, etc. The

green radiation can be produced by the downshifting process or by the upconversion process by NIR excitation. In the present work, Tb³⁺/Yb³⁺ ions doped self-activated LaNbO₄ phosphor sample have been synthesized through a solid-state reaction method by multiple heating at 1473 K. The XRD, SEM, EDS, and XPS techniques have been used for the structural analysis. The optical characterization was carried out by UV-VIS, FTIR, PLE, DS UC, and time-domain measurements. LaNbO₄:15Tb³⁺ phosphor samples emit intense green emission at 545 nm along with weak red on excitation with 262 nm charge transfer band (CTB) of [NbO₄]³⁻ and 378,486 nm (atomic line of Tb³⁺) respectively. The 262nm excitation also gives intense blue emission satisfying the white light emission condition. It is interesting that the multiple-time heating affects the energy transfer host to Tb³⁺. and the emitted downshifting green emission of Tb³⁺ ions in LaNbO₄ CIE color purity is high. The Tb³⁺/Yb³⁺ doped LaNbO₄ phosphor generates up conversion emission in the visible region through cooperative energy transfer. This sample also gives intense quantum cutting emission with the multiple-time heating of the phosphor. The energy level diagram can well understand the multi-mode emission behavior. Utilization of the intense green and NIR emission of this phosphor in various fields such as green laser, plasma display panels, UV sensors, photodynamic therapy, Cancer treatment, LEDs, solar cells, etc.

55. UPTAKE AND ACCUMULATION OF HEAVY METALS (PB & CR) BY SPINACH (*SPINACIA OLERACEA* L.) GROWN IN DIFFERENT SEWAGE IRRIGATED SOILS

Suraj Patel, Dinesh Mani, Jeetendra Verma, Manoj Kumar and Rupesh Kumar Ojha

Sheila Dhar Institute of Soil Science, Department of Chemistry, University of Allahabad, Prayagraj 11 002 (Uttar Pradesh), India

Email: sp358495@gmail.com

Abstract

The present study was carried out in order to observe the accumulation potential of Spinach (*Spinacia oleracea* L.) grown in different sewage irrigated sites in prayagraj U. P. Soil and plant samples were collected from various sewage irrigated sites viz. (Buxibandh, Preetam Nagar and Mehndauri) in Prayagraj. The *Spinacia oleracea* L. has showed that ability to accumulate the different concentrations of Pb & Cr ranged from (4.36±0.18 .09±0.10 and 3.67±0.21 .04±0.12 mg/kg) in root and (4.32±0.14 .11±0.13 and 3.71±0.12 .01±0.17 mg/kg) in shoot respectively. The results showed that maximum accumulation of Pb was observed in Buxibandh site followed by Cr, while the minimum accumulation of Pb and Cr in Mehndauri site. The maximum dry biomass yield of *Spinacia oleracea* L. plants were observed in Mehndauri polluted site with Pb and Cr recorded from (6.15±0.21 .67±0.18). While minimum dry biomass yield was observed (4.49±0.22 .08±0.27) from Pb and Cr polluted soils in Buxibandh site. Furthermore, their bioconcentration factor (BCF) and translocation factor (TF) >1.0 indicated that the hyper accumulation ability of *Spinacia oleracea* L. ranges of Pb and Cr was observed (0.68±0.012 .01±0.03) and (0.99±0.02 .00±0.14) respectively. Thus, these study findings underscore the need for monitoring sewage-irrigated agriculture practices to prevent heavy metal contamination in food chain and safeguard public health.

56. COMPACT PORTABLE INERTIAL ELECTROSTATIC CONFINEMENT FUSION NEUTRON SOURCE

Surender Kumar Sharma, Busam Partha Sashank, Rishu Kumar, G Kiran Kumar and Archana Sharma

Pulsed Power & Electromagnetic Division, Bhabha Atomic Research Center, Visakhapatnam

Homi Bhabha National Institute, Mumbai

Email : surender@barc.gov.in

Abstract

Inertial Electrostatic Confinement fusion neutron source in spherical & cylindrical configuration is designed and developed for activation analysis. The spherical Inertial Electrostatic Confinement device consists of spherical concentric inner cathode and outer anode grids of 30mm and 120mm diameters placed inside the vacuum chamber. The Inertial Electrostatic Confinement system is operated at a pressure of 0.01-0.06 mbar with deuterium gas medium. Proper insulation feed through is provided between cathode grid and outer chamber in order to prevent breakdown. The cylindrical Inertial Electrostatic Confinement source consists of two plate anodes of 80 mm diameter at both ends and a cylindrical cathode of 60 mm diameter in the center enclosed in a ceramic vacuum chamber of 450 mm length. The Inertial Electrostatic Confinement source was operated with deuterium gas at 0.01 – 0.06 mbar. High voltage of 25 – 30 kV is applied to the cathode grid with anode grounded and neutron yield of $>10^4$ n/s is measured from the spherical Inertial Electrostatic Confinement source, and neutron yield of $>10^5$ n/s is measured from the cylindrical Inertial Electrostatic Confinement source with He neutron flux monitor. The details of spherical and cylindrical Inertial Electrostatic Confinement neutron source, its construction, testing and operation are presented in this article.

57. HYDROTHERMALLY SYNTHESIZED IRREGULAR α - V_2O_5 NANODISCS FOR ROOM TEMPERATURE OPERABLE AMMONIA SENSOR

Surya Prakash Singh, Satyam Tripathi and Pratima Chauhan

Advanced Nanomaterials Research Laboratory, U.G.C. Centre of Advanced Studies, Department of Physics, University of Allahabad, Prayagraj 11002, India.

Centre of Material Sciences, IIDS, University of Allahabad, Prayagraj 11002, India.

Email: sps.phd2021@allduniv.ac.in, mangu167@yahoo.co.in*

Abstract

The current study explores the deployment of hydrothermally synthesized vanadium pentoxide (α - V_2O_5) irregular nanodiscs for ammonia (NH_3) detection at ambient temperature. Various investigations utilizing X-ray diffraction, UV-visible spectroscopy, FE-SEM, HR-TEM, and EDX mapping have been conducted on the prepared samples to evaluate their morphological and micro structural features. Utilizing the Debye-Scherrer equation, the crystallite size was determined to be 27 nm. It was found that the synthesized α - V_2O_5 sample was suitable for extremely sensitive chemiresistive ammonia sensors. A range of ammonia concentrations (50–500 ppm) were examined on the prepared sensor. The prepared sensor demonstrated exceptional

sensing capabilities towards NH_3 , with a response and recovery time of 22 s and 17 s respectively. Rising relative humidity (RH) just slightly reduced the sensor's response.

58. ABILITY OF NUMEROUS RECENT CHEMICAL AND PHYSICAL APPROACHES FOR THE ELIMINATION OF WASTEWATER DYE

Sapna Tomar and Swati Tomar

Department of Chemistry, Agra College Agra, Gautam Buddha University, Greater Noida

Email: sapnatomar_rbs@rediffmail.com

Abstract

Dye effluents emitted from a variety of dye-use industries are toxic to the atmosphere and to living things. As a consequence, the presence of dye effluent in environmental water sources is becoming an increasing issue. Environmentalists and the civilian community a long-term sustainable and effective method of treatment of dye effluents should be developed to resolve this problem. Until publication, dye wastewater should be processed first to mitigate the negative waste water impacts on the atmosphere and on living organisms. However, due to a lack of knowledge on efficient dye removal methods, it is difficult to settle on a single technique to address the prevailing dye effluent problem. Accordingly, this paper examines current study papers on different molecular, chemical and physical dye removal approaches in order to find their effectiveness by a percentage of dye removal. While there are several tried and tested current and the methods evaluated for the removal of pigment, most of which have a common drawback in the production of secondary emissions to the atmosphere. This paper illustrates the depletion of the enzyme (biological) and these days, adsorption (physical) dye removal is considered as one of the most effective dye removal techniques. This paper also recommends the use of a mixed adsorbent, since it is envisaged that this approach would be more effective and would be able to extract dyes at a quicker rate.

59. THE STRUCTURAL PROPERTIES OF ABX_3 FAMILY OF PEROVSKITES

T. Gayatri and Amar Kumar

Department of Physics, B. S. A. College, Mathura, India, 281004

Department of Physics, K. R. (P.G.) College, Mathura, (India), 281001

Email: kumarkrc@gmail.com

Abstract

The evaluation of these properties of new materials, Ionic radii, electronegativity and quantities are very useful parameters and the average ionic radii r_{av} of any compound is key parameter for calculating physical properties. In this paper, a simple model of structural property prediction based on ionic charge theory of solid is proposed. The structural property of tetragonal perovskites (lattice constant) exhibits a linear relationship against the average ionic radii r_{av} (\AA), alongwith the ionic charge product of the perovskite solids. This enables us to achieve improved prediction performance of the lattice constant of structurally known perovskites. We have applied the proposed relation to tetragonal perovskites and found a better agreement with the experimental data as compared to the values evaluated by earlier researchers.

60. ANALYTICAL TECHNIQUES FOR MEDICAL DEVICE EXTRACTABLES ANALYSIS

T.B.Patrudu, Tentu Nageswara Rao and Tentu Manohra Naidu

Department of Chemistry, GITAM University, Hyderabad Campus.

Department of Analytical Chemistry Harmoni Analyticals Pvt. Ltd, IDA Jeedimetla, Hyderabad, Telangana 500055.

Department of Physics, Raghu Engineering College, Dakamarri, Visakhapatnam, AP, India.

Email: patrudupath@gmail.com

Abstract

Mandible and maxilla bone loss is a significant challenge for plastic and reconstructive surgeons, causing aesthetic and functional defects. Current treatments involve autograft replacement and titanium dental implants. However, synthetic bone grafts have limitations for bone augmentation. Researchers have developed a regenerative bone graft called Nanocomposite Fibrous Scaffold for intraoral bone augmentation. This biomimetic, osteoconductive, porous, mechanically stable, and biodegradable device promotes new bone formation in critical mandible defects and integrates well with titanium dental implants. The test device will be placed in two solutions, purified water and hexane, to determine the amount of solution extracted and select a solvent. The solvent compatibility will be judged qualitatively, and samples will be extracted at 50 ± 2 °C for 72 ± 2 hours. Infrared analysis, GC-MS/MS, LC-MS/MS, and ICP-MS will be performed on the extract to identify volatile, semi-volatile, non-volatile organic compounds, and metals, comparing the results to a blank medium. The purpose of this test is to determine the extractables from the test item, "(Nanocomposite Fibrous Scaffold)" made up of Silica-nanohydroxyapatite-gelatin aligned with poly (L-lactoc acid) fibers using polar and non-polar solvents i.e. purified water and n-hexane respectively.

61. REDOX-ACTIVE POROUS ORGANIC POLYMERS FOR SODIUM-ION AND SODIUM DUAL-ION BATTERIES

Tapas Kumar Dutta, Suprabhat Sarkar and Abhijit Patra

Department of Chemistry, Indian Institute of Science Education and Research Bhopal,

M.P. 462066, India

Email: tapas17@iiserb.ac.in, abhijit@iiserb.ac.in

Abstract

Porous organic polymers have gained renewed interest as a promising electrode material for electrochemical energy storage, owing to their high specific surface area, abundant microporosity, tunable redox functionalities, and electrochemical stability.¹ At present, lithium-ion batteries (LIBs) are the state-of-the-art energy storage technology for portable electronics to electric vehicles.² However, the scarcity and uneven distribution of lithium resources on Earth result in increasing constraints on the use of lithium-ion batteries in the future. In this context, sodium-ion batteries (SIBs) are expected to be one of the promising alternatives to LIBs for powering up electric vehicles and large-scale grid energy storage due to the low cost and high natural abundance of sodium.² However, the challenge lies in achieving the desired electrochemical properties through precise structural modulation and the incorporation

of redox-active functional units. Our group is working on the development of redox-active organic anode materials for sodium-ion and sodium dual-ion batteries. In the first study, we developed a triptycene-based microporous organic ladder polymer featuring vertically aligned quinone moieties for high-performance SIBs.⁴ However, the low electrical conductivity of POPs often leads to inadequate electrochemical performance for metal-ion batteries. Thereafter, we developed a β -ketoenamine-linked covalent organic framework (COF), grown on multi-walled carbon nanotubes through *in situ* polycondensation method, which exhibits enhanced electrical conductivity of the COF composites with a high specific capacity and excellent cyclic stability. Further, we developed a triphenylamine-pyrene-based POP that could host the sodium and hexafluorophosphate ions simultaneously and could be used as both anode.

62. AN ASSESSMENT OF THE IMPACT OF TRIFLOXYSTROBIN 500 G/L SC ON THE SOIL MICROFLORA

Tentu Nageswara Rao and Pavan Kumar Kota

Department of Analytical Chemistry, Harmoni Analyticals Pvt. Ltd, IDA Jeedimetla, Hyderabad, Telangana 500055.

Email: tnraochemistry@gmail.com

Abstract

Trifloxystrobin, a fungicide, works against fungal pathogens by inhibiting mitochondrial respiration in fungi. It has a significant impact on soil microflora, which is important for nutrient cycling and soil health. Trifloxystrobin can influence soil microbial communities, potentially affecting beneficial mycorrhizal fungi and bacteria involved in nitrogen fixation or decomposition processes, potentially impacting soil fertility and plant health. The study evaluated the impact of trifloxystrobin on soil microflora through a nitrogen transformation and short-term respiration test, following OECD guidelines, following application to loamy sand soil. The study tested the effect of trifloxystrobin on soil nitrate content and respiration rates in loamy sand soil over 28 days. The concentrations of trifloxystrobin were 2 mg/kg soil dry weight and 10 mg/kg soil dry weight. The nitrate content deviations were 1.12%, 8.04%, and 13.26%, respectively. The rate of nitrate formation differed from controls by 21.14%, 9.19%, and 10.47% for the different concentrations. The respiration rates in trifloxystrobin treated soils were not statistically significantly different from control values. Deviations in nitrate levels, nitrate formation rates, and rates of short-term respiration in soil treated with up to and including trifloxystrobin were low and <25%, indicating no significant effect on carbon or nitrogen transformation.

63. HYDROGEN ENERGY: POTENTIAL SOLUTION TO ENVIRONMENTAL POLLUTION AND TRANSPORTATION PROBLEMS

Thakur Prasad Yadav

Department of Physics, Faculty of Science, University of Allahabad, Prayagraj 11002

Email: tpyadav@allduniv.ac.in

Abstract

Energy is an important part of human life; however, the world is facing an energy crisis due to exponential population growth and the limited availability of fossil fuels. It needs essential

attention with regard to its availability; therefore, solving this energy demand using more efficient or clean alternative energy sources will not only save the planet from harmful effects caused by pollution but could also reduce disparity and create a more peaceful world. For India, an increase in population is another reason for the increased demand for energy. Nanomaterials, one of the most important materials nowadays, such as nanoparticles, nanotubes, and 2D materials, have been proposed as catalysts for energy generation and storage because of their extraordinary properties and ease of production. Quasicrystals are complex in nature, having transition metal elements, and it has been difficult to gain an atomic-scale understanding of the catalytic activity of the quasicrystals. In order to achieve this information, we have attempted to create a simple model catalyst of a two-dimensional layer of nanoparticles on quasicrystalline surfaces by leaching well-defined surfaces of single-grain quasicrystals. As the first step of these studies, we present here the effect of leaching treatments on the surface morphology and chemical composition of different Al-based quasicrystals studied by scanning electron microscopy (SEM), energy dispersive x-ray (EDX) analysis, and x-ray photoelectron spectroscopy (XPS). The high-symmetry surfaces of single-grain icosahedral (i)-Al-Cu-Fe and decagonal (d)-Al-Ni-Co and (d)-Al-Cu-Co quasicrystals and a polygrain (i)-Al-Pd-Re, (i)-Al-Cu-Fe, and (i)-Al-Pd-Mn quasicrystal with random surface orientation were leached with NaOH solution at varying times, and the resulting surfaces were characterized by scanning electron microscopy, energy dispersive x-ray analysis, and x-ray photoelectron spectroscopy[1-4]. The leaching treatments preferentially remove Al-producing nanoparticles of the transition metals and their oxides. The leached fivefold surface of i-Al-Cu-Fe exhibits micron-sized dodecahedral cavities on which the nanoparticles are precipitated. However, no specific microstructure has been observed on the tenfold surface of d-Al-Ni-Co and the polygrain i-Al-Pd-Re. Quasicrystalline surfaces can be regained after polishing the leached layer, indicating that leaching occurs only at a limited depth from the surface. The use of such 2-D nanomaterials for hydrogen production will be discussed and presented in detail, explaining how their remarkable properties can enhance the efficiency of hydrogen production and storage. The 2-hour-leached as-grown and mechanically activated Al-Cu-Fe layer materials were subjected to catalyst application in hydrogen storage materials for MgH_2 . The catalytic effect of leached quasicrystalline and high entropy alloys on the de/rehydrogenation characteristics has been studied. The hydrogenation behavior, including absorption kinetics, will be discussed and presented in detail.

64. DESIGN, ADMET ANALYSIS, DOCKING, MOLECULAR DYNAMICS SIMULATIONS, SYNTHESIS AND ANTIVIRAL ACTIVITIES OF QUINOLINE DERIVATIVES AGAINST VARIOUS DNA/RNA VIRUSES

Vishal K. Singh, Shivangi Rai and Ramendra K Singh

Department of Chemistry, University of Allahabad, Prayagraj, India 11002

Email: rksingsrk@gmail.com

Abstract

A series of quinoline derivatives have been designed synthesized and screened for their broad spectrum anti-viral activity. Drug likeness properties of all the compounds were evaluated first, then these molecules were subjected to molecular docking and molecular dynamics (MD) simulations. Molecular docking simulation showed that all compounds form hydrogen bonds

with different types of amino acid residues Arg84, Met114, Phe126, Tyr89, Trp121, Asn115, Ile124, Ser152, Asn122, Ile124 etc. Antiviral screening of all the compounds indicates that compound 4 has excellent antiviral activity against Respiratory syncytial Virus (RSV) with a selectivity index (SI) of 11.6 and compound 6 is effective against Yellow Fever Virus (YFV) with a selectivity index of 28.5. Molecular dynamics simulation study was also performed on compound 4 and ribavirin with target protein (PDB ID: 6BLH), which reveals that the complex formed between compound 4 and target protein (PDB ID: 6BLH) was stable similar to the complex formed between the reference drug ribavirin and target protein (PDB ID: 6BLH).

65. SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL SCREENING OF 3- SUBSTITUTED ANTHRANILIC ACID OF MALEIMIDES

Yogeshwar R. Deokar, Keshao A. Mahale and Vivekanand B Jadhav

Department of Chemistry, Shri Muktanand College Gangapur, Dist-Aurangabad, Maharashtra, Pin-431109, India.

Department of Chemistry, Deogiri College, Aurangabad, Maharashtra, Pin- 431005, India.

Department of Chemistry, K. R. T. Arts, B. H. Commerce and A. M. Science College, Gangapur Road, Nashik-422 002, Maharashtra, India.

Email: viveka22@gmail.com

Abstract

N-substituted cyclic maleimides is a group of interested compounds due to their numerous applications in biology, pharmacology, synthetic chemistry, polymerchemistry, and material science. Maleimides also exist antibacterial, antitumor and tuberculostatic activity. Maleimide moiety is biological active due to presence of α , β -unsaturated carbonyl groups, two amide group and various substituents on Nitrogen atom. The biological activity can be enhanced by substituted various group at 3, 4 position or at Nitrogen.

Novel hybrid molecules containing cyclic maleimides and anthranilic acid moieties were efficiently synthesized and characterized by spectroscopic techniques such as IR, ^1H NMR, ^{13}C NMR, mass spectrometry. The synthesized molecules were screened for their antimicrobial activity against bacteria as well as fungal strains. The minimum inhibitory concentrations (MICs) were also determined. The investigation of antimicrobial screening data revealed that the most of the compounds exhibited moderate to good microbial activity.

66. DESIGN, SYNTHESIS, MOLECULAR DOCKING, MOLECULAR DYNAMICS AND CYTOTOXICITY OF NOVEL COUMARIN DERIVATIVES AS POTENTIAL INHIBITORS OF ACETYLCHOLINESTERASE

Shivangi Rai, Vishal K Singh, Yugandhar Maurya and Ramendra K. Singh

Bioorganic Research Laboratory, Department of Chemistry, University of Allahabad Prayagraj-211002, India

Email: rksinghsrk@gmail.com

Abstract

A series of novel coumarin derivatives has been meticulously designed and synthesised as potential AChE inhibitors against Alzheimer's disease. Firstly, the physicochemical parameters

and drug-like properties of all compounds were assessed followed by molecular docking and molecular dynamics simulation (MDS) targeting the active site of protein. Molecular docking analysis revealed that compounds had higher binding affinities and formed hydrogen bonds with Phe288, Tyr70, Tyr121, Asp72, Lys413, Gln69, Gln526 and Arg289 the highly conserved amino acids of the active site of the target protein. Several parameters like RMSD, RMSF, and RGyr of Molecular Dynamics Simulation (MDS) demonstrated stable interactions between compounds and target protein over a 100 ns period. Further, the cytotoxicity experiment against HEK293 cell lines revealed that several compounds maintained high cell viability at concentrations of 10, 20, 40, 80, and 90 $\mu\text{g/mL}$, indicating low toxicity. The results strongly supported the potential of these compounds to serve as effective inhibitors of the AChE enzyme.



The National Academy of Sciences, India (NASI), Prayagraj

📍 5, Lajpatrai Road,
Prayagraj - 211 002, India

☎ +91-532-2640224

✉ nasi.allahabad1@gmail.com

🌐 nasi.org.in



Indian Institute of Science Education and Research (IISER) Bhopal

📍 Bhopal Bypass Road, Bhauri Bhopal
462 066, Madhya Pradesh, INDIA

☎ 0755-269-2316

✉ office_director@iiserb.ac.in

🌐 iiserb.ac.in

