2nd International Conference on Recent Trends in Materials Science & Devices 2023 (ICRTMD-2023)

29 - 31 December, 2023

Online Conference https://www.rpconfseries.com/



e-Abstract Book

Jointly Organized by:

Research Plateau Publishers

(An academic publisher of scientific and technical journals)

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Sat Kabir Institute of Technology & Management, Bahadurgarh, Haryana (Affiliated to M.D. University, Rohtak, Haryana, India)





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About Conference

Aims:-

- To provide a platform for presenting research to an international and interdisciplinary audience.
- To help in establishing business or research relations and find global partners for future collaboration.
- The scientific programme will highlight the latest advances in materials research.
- To acquire deep theoretical and experimental knowledge from young researchers and experts.

Outcomes:-

- Exposure to International Research & Development.
- Opportunity to collaborate leading researchers around the globe.
- Full-length research papers will be published in Google Scholar Indexed Open Access Journals of Research Plateau Publishers and SCOPUS Indexed Journal Materials Protection (Publisher: Engineers Society of Corrosion, Belgrade).
- Proceedings of all abstracts will be published online.

Themes of Conference (but not limited to)

1. Material Properties and Characterization:

- Mechanical properties
- Electrical properties
- Thermal properties
- Optical properties
- Magnetic properties
- Chemical properties
- Rheological properties
- Surface properties

2. Materials Synthesis and Processing:

- Chemical synthesis
- Bulk material processing
- Thin film deposition
- Powder metallurgy
- Sol-gel processing
- Nanofabrication techniques
- Additive manufacturing (3D printing)
- Surface modification techniques

3. Material Selection and Design:

- Materials selection charts (e.g., Ashby charts)
- Design for specific properties
- Computational materials design
- Materials databases and informatics

4. Materials for Energy Applications:

- Solar cell materials
- Battery materials
- Fuel cell materials
- Thermoelectric materials
- Materials for energy storage and conversion

5. Electronic and Optoelectronic Materials:

- Semiconductors
- Superconductors
- Photonic materials
- Organic electronics
- Magnetic materials for data storage

6. Structural Materials:

- Metals and alloys
- Ceramics
- Polymers
- Composite materials
- Lightweight materials
- High-strength materials
- Corrosion-resistant materials

7. Biomedical Materials:

- Biomaterials
- Biocompatibility
- Tissue engineering scaffolds
- Drug delivery systems
- Dental materials
- Implants and prosthetics

8. Nanomaterials and Nanotechnology:

- Nanoparticles
- Nanotubes
- Nanocomposites
- Nanoelectronics
- Nanophotonics
- Nanomechanics
- Self-assembly

9. Advanced Characterization Techniques:

- Transmission electron microscopy (TEM)
- Scanning electron microscopy (SEM)
- X-ray diffraction (XRD)
- Nuclear magnetic resonance (NMR)
- Mass spectrometry (MS)
- Atomic force microscopy (AFM)
- X-ray photoelectron spectroscopy (XPS)

10. Smart and Responsive Materials:

- Shape memory alloys
- Hydrogels
- Piezoelectric materials
- Thermoresponsive materials
- pH-responsive materials
- Light-responsive materials

11. Environmental Sustainability:

- Green materials
- Recycling and upcycling
- Sustainable production methods
- Life cycle analysis
- Waste reduction

12. Materials for Extreme Conditions:

- High-temperature materials
- Radiation-resistant materials
- High-pressure materials
- Materials for space exploration

13. Emerging Materials:

- 2D materials (e.g., graphene)
- Topological materials
- Perovskite materials
- Quantum materials
- Metamaterials

14. Device Fabrication and Integration:

- Microfabrication
- MEMS (Microelectromechanical Systems)
- Semiconductor device manufacturing
- Integration of materials into devices

15. Materials for Information Technology:

Semiconductor materials

Spintronics materials

- Magnetic materials for data storage
- Photonic materials for communication

About Us

Research Plateau Publishers

Research Plateau Publishers is an academic publisher of scientific and technical journals. Our aim is to provide up-to-date scientific and technical achievement with high creativity and great significance on interdisciplinary and multidisciplinary platform for all the professionals to publish the research articles and to share knowledge for research studies. Our vision is to provide a one step solution for scientific and quality information. The main intention is to provide easy access of articles for all the Researchers, Scholars, Scientific Authors, Academic Societies, Professors, Lectures, Graduates, and Students.

We publish Original Research Articles, Short Research Articles, Short Communications, Review Articles, Mini Review Articles, Comments / Opinion Articles, Method Articles, Data Articles, Case Reports / Case Studies (Mainly for bio-medical journals), Clinical Practice Articles, Letter to the Editor, and Scholarly Book Review depending upon the scope and variety of a Journal.

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Website: https://researchplateau.com/

Sat Kabir Institute of Technology & Management, Bahadurgarh (Haryana)

Sat Kabir Institue of Technology & Management (SKITM) is spiritually oriented by Sat guru Sant GARIB DASS JI & Sat KABIR JI whose holy spirit may enlighten strength and guide for bright career of the students and the institution as a whole. SKITM is under the Trust "Sant Garib Dass Educational and charitable trust" Approved by AICTE and affiliated to Maharishi Dayanand University (M.D.U. Rohtak). The main aim of the trust is to provide opportunities of quality education to the talented students, particularly those belonging to underprivileged society to facilitate the attainment of national objectives of accelerating the process of modernisation.

Website: <u>https://skitm.edu.in/index.php</u>

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Guest of Honour Message

It is a matter of great pride and honor that Research Plateau Publishers and Sat Kabir Institute of Technology & Management, Bahadurgarh (Haryana), India are jointly organizing the "2nd International Conference on Recent Trends in Materials Science & Devices 2023 (ICRTMD 2023)" from December 29 to 31, 2023 in online mode.

The conference aims at providing a stimulating forum for eminent scholars from different branches of basic sciences: Physics, Chemistry, Statistics and Mathematics, and advancing the outcome of R&D in these areas from laboratory to practical devices, providing opportunity for the participants to interact with eminent researchers and to develop potential collaborative partnership. The conference also provides a forum for young aspirants to grow with their own start-ups for the overall development of research world.

Further, I am pleased to note that faculty and researchers from various reputed Universities, Colleges and Research Organizations across the globe are presenting their research papers on varied interdisciplinary topics of Materials Science & Engineering. I am sure that this International Conference would pave way for scientists, researchers, faculty members and young professionals which will unfold further opportunities and leads to new research developments.

I would like to commend the efforts put in by team ICRTMD 2023 and appreciate the invaluable contribution of all the lead speakers participating from India and abroad from scientific organizations and academia.

In the end, I wish ICRTMD 2023 a grand success.

Dr. Yogendra Kumar Mshra



Dr. Amrita Hooda Founder Research Plateau Publishers, Jhajjjar (Haryana), India



Organizing Secretary's Message

It is a great honour that Research Plateau Publishers and Sat Kabir Institute of Technology & Management, Bahadurgarh (Haryana), India are jointly organizing the "2nd International Conference on Recent Trends in Materials Science & Devices 2023 (ICRTMD 2023)" from December 29 to 31, 2023 in online mode.

The conference aims at providing a common forum for eminent scientists, technologists, entrepreneurs and scholars from various disciplines such as Physics, Chemistry, Material Science and Mathematics to present their work and discuss the latest advances and innovations in this exciting area of research.

When addressing societal challenges, the scientific world must strike the right balance between supporting research in all scientific areas and creating opportunities for both large-scale and small-scale projects that break through disciplinary boundaries. In the modern era, interdisciplinary research is the key to future innovations. From such funders to journal editors, policymakers to think tanks all seem to agree that the future of research lies outside firm disciplinary boundaries.

The "2nd International Conference on Recent Trends in Materials Science & Devices 2023 (ICRTMD 2023)" is being organized to bring together academicians, scientists and industrialists from various fields for the establishment of enduring connections to solve the common global challenges across a number of disciplines. The conference would be a platform to tackle complex problems from a range of perspectives, thereby modeling integrated, solution-focused thinking and partnerships.

I am sure that this conference would be thought provoking and lead to germination of new ideas.

I wish the conference a great success.

Dr. Amrita Hooda



Dr. H. K. Chhillar Chairman Sat Kabir Institue of Technology & Management, Bahadurgarh, Haryana, India



Convenor's Message

I greatly appreciate the untiring efforts from Research Plateau Publishers and Sat Kabir Institute of Technology & Management, Bahadurgarh (Haryana), India for jointly organizing the "2nd International Conference on Recent Trends in Materials Science & Devices 2023 (ICRTMD 2023)" from December 29 to 31, 2023 in online mode.

ICRTMD 2023 will provide a unique platform to all stakeholders to have intensive and brainstorming in the area. I extend my hearty welcome to all eminent speakers, distinguished subject experts and wrthy participants from various national and international universities, institutions and research establishments. I am sure that their deliberations on such an important area would pave the way for forging bonds and mutual cooperation, undertaking joint projects and joint publications for achieving long-term goals and establishing significant and long-term contacts for mutual benefits. It will be an enriching experience for brilliant faculty members, scientists, research scholars and students and other participants.

I extend my sincere appreciation to all distinguished members of International/National Advisory Committee for their valuable guidance. I extend a warm welcome to all the participants of ICRTMD 2023 and convey my best wishes for the success of the event.

Dr. H.K. Chillar



Dr. Rajeev Goyal

Associate Professor Sat Kabir Institue of Technology & Management, Bahadurgarh, Haryana, India



Co-Convenor's Message

I sincerely thank Research Plateau Publishers and Sat Kabir Institute of Technology & Management, Bahadurgarh (Haryana), India for their tireless efforts in organizing the online "2nd International Conference on Recent Trends in Materials Science & Devices 2023 (ICRTMD 2023)" from December 29 to December 31, 2023.

ICRTMD 2023 will give everybody with an interest an unique place for in-depth discussions and brainstorming in the field. I extend a warm welcome to all of the distinguished speakers, distinguished academic experts, and worthy attendees from different national and international universities, organizations, and research establishments. In order to achieve long-term objectives, I'm confident that their discussions on this key subject will open the door for them to collaborate and form bonds, work together on projects and publications, and build meaningful, long-lasting goals that will benefit all of them. For the brilliant faculty members, scientists, research experts, students, and other attendees, it will be a rewarding event.

I would like to express my profound gratitude to all of the esteemed members of the International/National Advisory Committee for their invaluable guidance. I welcome each and every one of the ICRTMD 2023 participants with great warmth and express my best wishes for the event's success.

Kgun

Dr. Rajeev Goyal

Contents

Keynote Talks			
Authors	Paper ID	Title	Page No.
Raman Singh	ICRTMD- 2023/KT/001	Success in Developing CVD Graphene Coating on Mild Steel for Remarkable Corrosion Resistance	1
S. K. Ghoshal	ICRTMD- 2023/KT/002	Improved Performance of Rose Bengal Dye- Encapsulated Plasmonic Au Nanoparticles- based Fiber-Optic Humidity Sensor	2
Anand P Pathak	ICRTMD- 2023/KT/003	Ion beams, Lasers and Gamma Radiations in Nano Science and Nano Technology	3
Manjeet Singh Goyat	ICRTMD- 2023/KT/004	Oxide nanoparticles reinforced polymer nanocomposites for advanced applications	4
Yogendra Kumar Mishra	ICRTMD- 2023/KT/005	Tetrapods based Smart Materials for Advanced Technologies	5
Surender Duhan, Bhavna, Supriya Sehrawat, Aryan Boora, Priya, Anisha, Sushma	ICRTMD- 2023/KT/006	Mesoporous Materials in Sensing Applications	6
Rehan Khan	ICRTMD- 2023/KT/007	NanoBiomaterials for the Therapy of Experimental Inflammatory Arthritis	7
Indra Sulania, Ambuj Tripathi, Ranjeet K Karn, Elham Chamanehpour, Ajani Lakmini Jayarathna, Y K Mishra	ICRTMD- 2023/KT/008	Applications of Zinc oxide Tetrapods based composites in Environmental Remediation	8
Santanu Ghosh	ICRTMD- 2023/KT/009	Miniaturized electron source with low dimensional materials: Emerging applications	9
Arif Kösemen'	ICRTMD- 2023/KT/010	Strategies for Lowering Operation Voltage of Organic Field Effect Transistors	10
Vinod Kumar	ICRTMD- 2023/KT/011	Nnano-Magnetic Oxide Particles and Fluids: Small Size – Vast Applications	11

Faculty/ Scientist (Invited) Talks

			1
Ashwani Kumar Sood	ICRTMD-	Impact of various co-solvents on the micellar	12
	2023/FIT/SIT/101	behavior of ionic surfactants	
Zeenat Arif	ICRTMD-	Mathematical modeling for the assessment of	13
	2023/FIT/SIT/102	antifouling property of biogenic synthesized	
		nanocomposite film	
Dr. L. Arunraja	ICRTMD-	Tuning Gas Sensing Properties in Chemically	14
	2023/FIT/SIT/103	Synthesized Zinc Oxide-Doped Cadmium	
		Sulfide Nanocomposites through Annealing	
		Effects	
Manash Jyoti Deka	ICRTMD-	Investigating optical properties of biomass waste	15
-	2023/FIT/SIT/104	derived carbon quantum dots prepared by	
		hydrothermal method	
Dan Bahadur Pal	ICRTMD-	Synthesis and Characterization of Copper Ceria	16
	2023/FIT/SIT/106	Oxide Nanofibers for Catalyst & Wastewater	
		Treatment	
Dr. Asim Kumar Roy	ICRTMD-	Synthetic Textile Polymers and Their	17
Choudhury	2023/FIT/SIT/108	Modifications	
Madhulata Shukla	ICRTMD-	DFT Study of Molecular Interaction of	18
	2023/FIT/SIT/110	Curcumin with Silver Nanocluster	
Chetan Chauhan	ICRTMD-	A Novel Spectrophotometric Method for Rapid	19
	2023/FIT/SIT/116	Quantification of Oseltamivir Phosphate Using	
		Dithiocarbamate Complexation	

Manvendra Kumar, Aartee Sharma, Parasmani Rajput	ICRTMD- 2023/FIT/SIT/117	X-ray Absorption Spectroscopy (XAS) for the local structure determination of nano- dimensional materials	20
Sucheta Sengupta, Rinki Aggarwal	ICRTMD- 2023/FIT/SIT/118	Fabrication of metal chalcogemide /p-Si NW heterostructured thin films for advanced	21
Kifayat H. Mir, Tarun Garg	ICRTMD- 2023/FIT/SIT/120	Resistive Switching in RF-Sputtered HfOx Based Random Access Memories with Low	22
Mahatta Oza, P.D.Solanki, M.J. Joshi	ICRTMD- 2023/FIT/SIT/121	Photocatalytic application and Cyclic Voltammetry Study of Nickel Pyrophosphate Nano-Particles	23
Rishi Pal	ICRTMD- 2023/FIT/SIT/124	Reduction in Environmental Electromagnetic Pollution using Conjugated Polymers	24
Kumar Gaurav	ICRTMD- 2023/FIT/SIT/127	Catalyzing Sustainability: Transesterification with Heterogeneous Catalysts forefficientBiodiesel Production	25
Aman Shukla, Sachin Kumar, Priyank Purohit	ICRTMD- 2023/FIT/SIT/128	Polyscharide polymer-linked Barium sulphate nano material for selective tumor cell diagnosis and treatment	26
Bijan Kumar Gangopadhyay	ICRTMD- 2023/FIT/SIT/129	Exploring a Spectrum of Size and Shape Effects: Melting Point and Lattice Parameter Dependencies in Gold and Copper Nanoparticles	27
Diptonil Banerjee	ICRTMD- 2023/FIT/SIT/130	Defect Rich Carbon Nanostructures Based Hybrids: Possible Cold Cathodes in Electron Microscope	28
Dr. Malay K Das	ICRTMD- 2023/FIT/SIT/131	Potential of Pharmaceutical Nanotechnology in the management of Neuro AIDS	29
Prasun Mukherjee	ICRTMD- 2023/FIT/SIT/133	Guiding Selection of Correct Ingredients to Realize Host Sensitized Dopant Emission	30
Priyanka Singh, Meena Choudhary	ICRTMD- 2023/FIT/SIT/134	Valorization of Dried Flowers of Medicinal Plant into Natural Dve	31
Madan Lal, Kamal Kishore, Navdeen Sharma	ICRTMD- 2023/FIT/SIT/136	Sol-gel derived Fe-doped ZnO NPs: Structural, Morphological and Magnetic Properties	32
Suma ND, Sari R Pillai	ICRTMD- 2023/FIT/SIT/143	Conductometric method for the determination of corrosion of Aluminium metal in hydrochloric acid medium	33
Rishibrind Kumar Upadhyay	ICRTMD- 2023/FIT/SIT/144	Solution-processed UV-visible-Near Infrared (NIR) broadband Photodetector based on ZnO/CH ₂ NH ₂ PbI ₂ heterojunction	34
Ravi Shankar Rai, Vivek Bajpai	ICRTMD- 2023/FIT/SIT/145	Development of metal-oxide nanostructured interphase in basalt fiber reinforced polymer composites for structural applications	35
Manorama Singh	ICRTMD- 2023/FIT/SIT/147	Nanomaterials-based Electrochemical Sensors for p-Phenylenediamine (An organic dye)	36
Dimpi Paul	ICRTMD- 2023/FIT/SIT/150	Displacement Sensor by Conventional Optical Fiber with Different Reflectometer for dissimilar Media	37
Dr. Sonali Bhatnagar	ICRTMD- 2023/FIT/SIT/154	Polumer Based Detectors Throw Light on Astroparticle Physics and Medical Physics	38
Richa Srivastava	ICRTMD- 2023/FIT/SIT/156	Synthesis of Proton Exchange Membranes for Microbial Fuel Cell	39
M. Pradeepa, D. Illakkiam, N. Geetha	ICRTMD- 2023/FIT/SIT/165	Green Synthesis and Photocatalytic Activity of Chitosan coated Iron Oxide Nanoparticles	40
Dr. M. Razia	ICRTMD- 2023/FIT/SIT/167	Biosynthesis of Silver Nanoparticles Using Psidium cattleianum Leaf extract and their Antimicrobial activity	41
Nitu Katariya, Ratnawali Verma, Pragya Agar Palod, R. Venkatesh, V.Ganesan	ICRTMD- 2023/FIT/SIT/176	Effect of doping on CuCrO ₂ prepared by solid state reaction method	42
Sayan Bayan	ICRTMD- 2023/FIT/SIT/178	Development of Triboelectric Nanogenerators for self-powered sensing application	43

Prithiviraj Khakhlary, Uddit Narayan Hazarika, Jhorna Borah, Arobinda Kakoti,	ICRTMD- 2023/FIT/SIT/179	3-D conductive metal organic frameworks (MOFs): Next generation conductive materials	44
Rinki Brahm, Kangkan Sarmah, Ankur Kanti Guba			
Jyoti Prakash Singh, Jyoti Srivastava, Mayank Dwivedi	ICRTMD- 2023/FIT/SIT/181	Experimental Investigation of Optical and Nanocooling Features of Silver Nanoparticles- Graphene Hybrid Material	45
Jesly Jacob, Simitha S, Devika Mohan, Vibin Ipe Thomas	ICRTMD- 2023/FIT/SIT/183	High-Performance SERS Substrates for Biomolecular Detections	46
K. Prabha	ICRTMD- 2023/FIT/SIT/184	Structural, Optical and Magnetic Properties of Transition metals doped Metal Oxide Nanoparticles	47
Anji Reddy Polu, Aseel A. Kareem, Hussein Kh. Rasheed	ICRTMD- 2023/FIT/SIT/186	Effect of POSS Hybrid Nanomaterials and MXenes on Solid Polymer Electrolytes for Rechargeable Lithium Batteries	48
Rubiya Samad, Saima Jahan	ICRTMD- 2023/FIT/SIT/187	Temperature dependent electric and magnetic properties of Pr doped BTO-NFO core-shell multiferroic nanocomposite	49
K. Nomita Devi, L. Anju Chanu	ICRTMD- 2023/FIT/SIT/189	Enhanced Photocatalytic Activity of Gd ³⁺ Doped ZnO Nanoparticles for Malachite Green Dye Degradation	50
Sigamani Saravanan, Raghvendra S. Dubey	ICRTMD- 2023/FIT/SIT/190	Silicon nitride (Si ₃ N ₄) anti-reflection coating thin film on silicon using chemical vapor deposition (CVD) techniques	51
Ashok Kumar	ICRTMD- 2023/FIT/SIT/200	Sol-Gel Synthesis of La-SnO ₂ NPs for Efficient Removal of dyes in Wastewater Treatment	52
Saroj Rani	ICRTMD- 2023/FIT/SIT/202	Methodology used for crystallization kinetics, optical properties and electrical behavior of heavy metal doped glasses	53
Debasree Saha	ICRTMD- 2023/FIT/SIT/204	Potential of solid supported copper catalyst in sustainable organic synthesis	54
Pratibha Kumari	ICRTMD- 2023/FIT/SIT/205	Synthesis of cellulose-based materials for sensing and environmental remediation	55
Ranimol Stephen	ICRTMD- 2023/FIT/SIT/206	Polymer Membranes for Separation Application	56
Nayan Mani Das	ICRTMD- 2023/FIT/SIT/208	Kelvin Probe Force Microscopy (KPFM) study on Antibacterial Behaviour of Graphene Oxide nanohybrid	57
Anand Kumar, Sushil Kumar	ICRTMD- 2023/FIT/SIT/211	Structural and Electrical changes investigations in aged copper sulphate doped poly (o-toluidine)	58
Priyanka Chhabra, Amit Tyagi	ICRTMD- 2023/FIT/SIT/215	Augmented healing of full thickness chronic excision wound by antimicrobial loaded chitosan encapsulated graphene nanocomposite	59
Anita Gupta, Rohit Babu Aniyery, Harminder Kaur	ICRTMD- 2023/FIT/SIT/216	Antimicrobial, anti-fungal and anticancer activity of N-(5-(N-((Z)-2-((Z)-(((5-acetamido- 1,3,4-thiadiazol-2-yl)sulfonyl)imino)methyl)-6- methoxyphenoxy)dioctylstannyl)oxy)-3- methoxybenzylidene)sulfamoyl)-1,3,4- thiadiazol-2-yl)acetamide	60
Subhasis Roy	ICRTMD- 2023/FIT/SIT/218	Architecture of inorganic-organic hybrid perovskites for enhanced stable photovoltaic performance	61
Indranil Maity, Aritra Chakrabarty	ICRTMD- 2023/FIT/SIT/221	Cadence Virtuoso Based Circuit Simulation of Universal Logic Gates: A Broad Tutorial	62
Naveen Kumari, Vinod Kumar	ICRTMD- 2023/FIT/SIT/225	Structural, Dielectric and magnetic studies on Al^{3+} substituted $ZnAl_{*}Fe_{2*}O_{4}$ ferrites	63
Mohammad Amir, Roohi	ICRTMD- 2023/FIT/SIT/226	Utilization of agro-wastes as solid substrate for biodegradable PHB production using microbes for sustainable environment	64
Aman Sen, Rajni, Ritika,	ICRTMD-	Role of Nd ³⁺ substitution on structural behaviour	65

Monokomno Surindor Doul	2023/FIT/SIT/227	of Bi _{1-x} Nd _x MnO ₃	
Manokannia, Sunneel Paul	ICDTMD	Develutionining illumination officiances in	66
Suresh Kumar Jakka, Pavam	ICKIMD-	keyolutionizing infumination efficiency in	00
Krisnnapuram	2023/F11/S11/228	metal-doped Phosphors	
Umesh Kumar	ICRTMD-	Exploration of cost effective earth-abundant	67
	2023/FIT/SIT/231	metals for enhanced electrocatalytic oxygen	
		evolution reaction	
Tripti Richhariya, Nameeta	ICRTMD-	Exploring the applicability of phosphors in	68
Brahme	2023/FIT/SIT/232	various fields	
Mridushmita Baruah, Dipak	ICRTMD-	Photocatalytic degradation of Phenol wastewater	69
Sinha	2023/FIT/SIT/235	by co-doped TiO2 activated carbon	
		nanocomposite	
S.S. Sarangi	ICRTMD-	Estimation of Glass Forming Ability and	70
C C	2023/FIT/SIT/236	Mechanical Properties of AlZr3 alloy using	
		Molecular Dynamics Simulations	
T. Mahalakshmi	ICRTMD-	Numerical Analysis of Convection of	71
	2023/FIT/SIT/237	Nanofluids on Heat Transfer – An Overview	
Meera R Gumaste	ICRTMD-	Comparative Study of Electrical Parameters of	72
	2023/FIT/SIT/240	Cadmium Telluride and Zinc Telluride	-
	2020/11/011/210	Nanoparticles by van der Pauw Hall	
		Measurements	
Sandinan Chatteriee Navan	ICRTMD-	A simple scalable transformation of waste laser	73
Sarkar Sumit Mandal Murali	2023/FIT/SIT/241	toper powder into the magnetic pigment for the	15
Sathish	2023/111/011/241	development of magnetic leather finishing: An	
Saunsn		innovative waste utilization strategy	
Monika Tomar	ICPTMD	L amb wave based acoustic devices for wireless	74
Wollika Tolliai	2023/FIT/SIT/243	sensing applications	/4
Poonam Kumari Gautam	ICRTMD-	Influence of Rotational Effects of Natural	75
I oonanii Kumari Oautam	2023/FIT/SIT/246	Convection Embedded by Jeffrey Nanofluid	15
	2023/11/011/210	Sheet in High Porosity	
Soumva Mukheriee Atiar	ICRTMD-	Synthesis characterization of Sodium Niobate	76
Rahaman Molla	2023/FIT/SIT/249	based Glass-	/0
Kulullull Monu	2023/11/011/21/	Ceramics for Energy applications	
Pranoti Kamble, C D	ICRTMD-	Quantum Dot Based Fluorescent Biosensing	77
Lokhande Arnita Pandey	2023/FIT/SIT/250	Device for early screening and detection of	
Tiwari Dr. Arpita Pandey	2023/11/011/230	cancer biomarkers	
Tiwari			
Swaroon K	ICRTMD-	Synthesis of Hydrogel Nanocomposites by	
Swaroop K			78
	2023/FIT/SIT/252	Radiation Assistance for Biomedical	78
	2023/FIT/SIT/252	Radiation Assistance for Biomedical	78
Mainak Ghosal	2023/FIT/SIT/252	Radiation Assistance for Biomedical Applications	78
Mainak Ghosal	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253	Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica	78 79
Mainak Ghosal	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD-	By Intests of Hydroger Autocomposites by Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica Influence of size and composition on	78 79 80
Mainak Ghosal Jyoti Dutta, Sourav Saikia, Saveed Ashigue Ahmed	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD- 2023/FIT/SIT/255	By Intests of Hydroger Autocomposites by Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica Influence of size and composition on fluorescence properties of carbonaceous	78 79 80
Mainak Ghosal Jyoti Dutta, Sourav Saikia, Sayeed Ashique Ahmed, Puspendu K Das	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD- 2023/FIT/SIT/255	By intests of Hydroger Autocomposites by Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica Influence of size and composition on fluorescence properties of carbonaceous nanoparticles (CNPs)	78 79 80
Mainak Ghosal Jyoti Dutta, Sourav Saikia, Sayeed Ashique Ahmed, Puspendu K. Das	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD- 2023/FIT/SIT/255	By intests of Hydroger Autocomposites by Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica Influence of size and composition on fluorescence properties of carbonaceous nanoparticles (CNPs) Ecofricandly and sustainiable panomaterials for	78 79 80
Mainak Ghosal Jyoti Dutta, Sourav Saikia, Sayeed Ashique Ahmed, Puspendu K. Das Jyoti Sharma, Monika Shukla, Subbasha Nigam	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD- 2023/FIT/SIT/255 ICRTMD- 2023/FIT/SIT/258	By intests of Hydroger Autocomposites by Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica Influence of size and composition on fluorescence properties of carbonaceous nanoparticles (CNPs) Ecofriendly and sustainiable nanomaterials for the ramoval of bazardous contaminants from	78 79 80 81
Mainak Ghosal Jyoti Dutta, Sourav Saikia, Sayeed Ashique Ahmed, Puspendu K. Das Jyoti Sharma, Monika Shukla, Subhasha Nigam, Monika Loshi	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD- 2023/FIT/SIT/255 ICRTMD- 2023/FIT/SIT/258	By intrests of Hydroger Autocomposites by Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica Influence of size and composition on fluorescence properties of carbonaceous nanoparticles (CNPs) Ecofriendly and sustainiable nanomaterials for the removal of hazardous contaminants from wasterwater	78 79 80 81
Mainak Ghosal Jyoti Dutta, Sourav Saikia, Sayeed Ashique Ahmed, Puspendu K. Das Jyoti Sharma, Monika Shukla, Subhasha Nigam, Monika Joshi Krishpaprahba Mapala	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD- 2023/FIT/SIT/255 ICRTMD- 2023/FIT/SIT/258	Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica Influence of size and composition on fluorescence properties of carbonaceous nanoparticles (CNPs) Ecofriendly and sustainiable nanomaterials for the removal of hazardous contaminants from wastewater Synthesis of Silver and Gold Nanoparticles	78 79 80 81
Mainak Ghosal Jyoti Dutta, Sourav Saikia, Sayeed Ashique Ahmed, Puspendu K. Das Jyoti Sharma, Monika Shukla, Subhasha Nigam, Monika Joshi Krishnaprabha Mapala	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD- 2023/FIT/SIT/255 ICRTMD- 2023/FIT/SIT/258 ICRTMD- 2023/FIT/SIT/259	By introses of Hydroger Autocomposites by Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica Influence of size and composition on fluorescence properties of carbonaceous nanoparticles (CNPs) Ecofriendly and sustainiable nanomaterials for the removal of hazardous contaminants from wastewater Synthesis of Silver and Gold Nanoparticles using Syzygium samarangense Fruit Extract as	78 79 80 81 82
Mainak Ghosal Jyoti Dutta, Sourav Saikia, Sayeed Ashique Ahmed, Puspendu K. Das Jyoti Sharma, Monika Shukla, Subhasha Nigam, Monika Joshi Krishnaprabha Mapala	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD- 2023/FIT/SIT/255 ICRTMD- 2023/FIT/SIT/258 ICRTMD- 2023/FIT/SIT/259	By introses of Hydroger Autocomposites by Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica Influence of size and composition on fluorescence properties of carbonaceous nanoparticles (CNPs) Ecofriendly and sustainiable nanomaterials for the removal of hazardous contaminants from wastewater Synthesis of Silver and Gold Nanoparticles using Syzygium samarangense Fruit Extract as Paducing Agent	78 79 80 81 82
Mainak Ghosal Jyoti Dutta, Sourav Saikia, Sayeed Ashique Ahmed, Puspendu K. Das Jyoti Sharma, Monika Shukla, Subhasha Nigam, Monika Joshi Krishnaprabha Mapala	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD- 2023/FIT/SIT/255 ICRTMD- 2023/FIT/SIT/258 ICRTMD- 2023/FIT/SIT/259	By introses of Hydroger Autocomposites by Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica Influence of size and composition on fluorescence properties of carbonaceous nanoparticles (CNPs) Ecofriendly and sustainiable nanomaterials for the removal of hazardous contaminants from wastewater Synthesis of Silver and Gold Nanoparticles using Syzygium samarangense Fruit Extract as Reducing Agent Advancements in Electrode Metarials for	78 79 80 81 82 83
Mainak Ghosal Jyoti Dutta, Sourav Saikia, Sayeed Ashique Ahmed, Puspendu K. Das Jyoti Sharma, Monika Shukla, Subhasha Nigam, Monika Joshi Krishnaprabha Mapala D. Saritha, R. Sujithra	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD- 2023/FIT/SIT/255 ICRTMD- 2023/FIT/SIT/258 ICRTMD- 2023/FIT/SIT/259 ICRTMD- 2023/FIT/SIT/259	Bynnesis of Hydroger Autocomposites by Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica Influence of size and composition on fluorescence properties of carbonaceous nanoparticles (CNPs) Ecofriendly and sustainiable nanomaterials for the removal of hazardous contaminants from wastewater Synthesis of Silver and Gold Nanoparticles using Syzygium samarangense Fruit Extract as Reducing Agent Advancements in Electrode Materials for Lithium-Ion Batteriae: A Comprehensive Study	78 79 80 81 82 83
Mainak Ghosal Jyoti Dutta, Sourav Saikia, Sayeed Ashique Ahmed, Puspendu K. Das Jyoti Sharma, Monika Shukla, Subhasha Nigam, Monika Joshi Krishnaprabha Mapala D. Saritha, R. Sujithra	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD- 2023/FIT/SIT/255 ICRTMD- 2023/FIT/SIT/258 ICRTMD- 2023/FIT/SIT/259 ICRTMD- 2023/FIT/SIT/262	By Intests of Hydroger Autocomposites by Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica Influence of size and composition on fluorescence properties of carbonaceous nanoparticles (CNPs) Ecofriendly and sustainiable nanomaterials for the removal of hazardous contaminants from wastewater Synthesis of Silver and Gold Nanoparticles using Syzygium samarangense Fruit Extract as Reducing Agent Advancements in Electrode Materials for Lithium-Ion Batteries: A Comprehensive Study	78 79 80 81 82 83 84
Mainak Ghosal Jyoti Dutta, Sourav Saikia, Sayeed Ashique Ahmed, Puspendu K. Das Jyoti Sharma, Monika Shukla, Subhasha Nigam, Monika Joshi Krishnaprabha Mapala D. Saritha, R. Sujithra Jyoti Katyal	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD- 2023/FIT/SIT/255 ICRTMD- 2023/FIT/SIT/258 ICRTMD- 2023/FIT/SIT/259 ICRTMD- 2023/FIT/SIT/262 ICRTMD- 2023/FIT/SIT/263	By adiation Assistance for Biomedical ApplicationsBehaviour of Cementitious Systems on Additions of Nano SilicaInfluence of size and composition on fluorescence properties of carbonaceous nanoparticles (CNPs)Ecofriendly and sustainiable nanomaterials for the removal of hazardous contaminants from wastewaterSynthesis of Silver and Gold Nanoparticles using Syzygium samarangense Fruit Extract as Reducing AgentAdvancements in Electrode Materials for Lithium-Ion Batteries: A Comprehensive StudyMagnetoplasmon Core shell Nanostructure	78 79 80 81 82 83 84
Mainak Ghosal Jyoti Dutta, Sourav Saikia, Sayeed Ashique Ahmed, Puspendu K. Das Jyoti Sharma, Monika Shukla, Subhasha Nigam, Monika Joshi Krishnaprabha Mapala D. Saritha, R. Sujithra Jyoti Katyal Dr. Saiid Babu Nalakatha	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD- 2023/FIT/SIT/255 ICRTMD- 2023/FIT/SIT/258 ICRTMD- 2023/FIT/SIT/259 ICRTMD- 2023/FIT/SIT/262 ICRTMD- 2023/FIT/SIT/263 ICRTMD-	Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica Influence of size and composition on fluorescence properties of carbonaceous nanoparticles (CNPs) Ecofriendly and sustainiable nanomaterials for the removal of hazardous contaminants from wastewater Synthesis of Silver and Gold Nanoparticles using Syzygium samarangense Fruit Extract as Reducing Agent Advancements in Electrode Materials for Lithium-Ion Batteries: A Comprehensive Study Magnetoplasmon Core shell Nanostructured Band-gap Engineering of Nanostructured CdSe-	78 79 80 81 82 83 84 85
Mainak Ghosal Jyoti Dutta, Sourav Saikia, Sayeed Ashique Ahmed, Puspendu K. Das Jyoti Sharma, Monika Shukla, Subhasha Nigam, Monika Joshi Krishnaprabha Mapala D. Saritha, R. Sujithra Jyoti Katyal Dr. Sajid Babu Nalakatha, Dr. M. Abdul Khadar	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD- 2023/FIT/SIT/255 ICRTMD- 2023/FIT/SIT/258 ICRTMD- 2023/FIT/SIT/259 ICRTMD- 2023/FIT/SIT/262 ICRTMD- 2023/FIT/SIT/263 ICRTMD- 2023/FIT/SIT/266	Bytational Systems of Hydrogen Autocomposition by Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica Influence of size and composition on fluorescence properties of carbonaceous nanoparticles (CNPs) Ecofriendly and sustainiable nanomaterials for the removal of hazardous contaminants from wastewater Synthesis of Silver and Gold Nanoparticles using Syzygium samarangense Fruit Extract as Reducing Agent Advancements in Electrode Materials for Lithium-Ion Batteries: A Comprehensive Study Magnetoplasmon Core shell Nanostructure Band-gap Engineering of Nanostructured CdSe-Cu-Se Thin Films	78 79 80 81 82 83 84 85
Mainak Ghosal Jyoti Dutta, Sourav Saikia, Sayeed Ashique Ahmed, Puspendu K. Das Jyoti Sharma, Monika Shukla, Subhasha Nigam, Monika Joshi Krishnaprabha Mapala D. Saritha, R. Sujithra Jyoti Katyal Dr. Sajid Babu Nalakatha, Dr. M. Abdul Khadar Pranati Purobit	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD- 2023/FIT/SIT/255 ICRTMD- 2023/FIT/SIT/258 ICRTMD- 2023/FIT/SIT/259 ICRTMD- 2023/FIT/SIT/262 ICRTMD- 2023/FIT/SIT/263 ICRTMD- 2023/FIT/SIT/266 ICRTMD-	Bytatistics of Hydroger Autocomposites by Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica Influence of size and composition on fluorescence properties of carbonaceous nanoparticles (CNPs) Ecofriendly and sustainiable nanomaterials for the removal of hazardous contaminants from wastewater Synthesis of Silver and Gold Nanoparticles using Syzygium samarangense Fruit Extract as Reducing Agent Advancements in Electrode Materials for Lithium-Ion Batteries: A Comprehensive Study Magnetoplasmon Core shell Nanostructure Band-gap Engineering of Nanostructured CdSe-Cu ₂ Se Thin Films Moving from Ph to Ph- Free Piezoceramics: A	78 79 80 81 82 83 84 85 86
Mainak GhosalJyoti Dutta, Sourav Saikia, Sayeed Ashique Ahmed, Puspendu K. DasJyoti Sharma, Monika Shukla, Subhasha Nigam, Monika JoshiKrishnaprabha MapalaD. Saritha, R. SujithraJyoti KatyalDr. Sajid Babu Nalakatha, Dr. M. Abdul KhadarPranati Purohit	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD- 2023/FIT/SIT/255 ICRTMD- 2023/FIT/SIT/258 ICRTMD- 2023/FIT/SIT/259 ICRTMD- 2023/FIT/SIT/262 ICRTMD- 2023/FIT/SIT/263 ICRTMD- 2023/FIT/SIT/266 ICRTMD- 2023/FIT/SIT/269	By Intests of Hydroger Autocomposites by Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica Influence of size and composition on fluorescence properties of carbonaceous nanoparticles (CNPs) Ecofriendly and sustainiable nanomaterials for the removal of hazardous contaminants from wastewater Synthesis of Silver and Gold Nanoparticles using Syzygium samarangense Fruit Extract as Reducing Agent Advancements in Electrode Materials for Lithium-Ion Batteries: A Comprehensive Study Magnetoplasmon Core shell Nanostructure Band-gap Engineering of Nanostructured CdSe-Cu ₂ Se Thin Films Moving from Pb to Pb- Free Piezoceramics: A Review	78 79 80 81 82 83 84 85 86
Mainak Ghosal Jyoti Dutta, Sourav Saikia, Sayeed Ashique Ahmed, Puspendu K. Das Jyoti Sharma, Monika Shukla, Subhasha Nigam, Monika Joshi Krishnaprabha Mapala D. Saritha, R. Sujithra Jyoti Katyal Dr. Sajid Babu Nalakatha, Dr. M. Abdul Khadar Pranati Purohit S C Rakesh Roshan. N	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD- 2023/FIT/SIT/255 ICRTMD- 2023/FIT/SIT/258 ICRTMD- 2023/FIT/SIT/259 ICRTMD- 2023/FIT/SIT/262 ICRTMD- 2023/FIT/SIT/263 ICRTMD- 2023/FIT/SIT/266 ICRTMD- 2023/FIT/SIT/269 ICRTMD-	By Intests of Hydroger Autocomposites by Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica Influence of size and composition on fluorescence properties of carbonaceous nanoparticles (CNPs) Ecofriendly and sustainiable nanomaterials for the removal of hazardous contaminants from wastewater Synthesis of Silver and Gold Nanoparticles using Syzygium samarangense Fruit Extract as Reducing Agent Advancements in Electrode Materials for Lithium-Ion Batteries: A Comprehensive Study Magnetoplasmon Core shell Nanostructure Band-gap Engineering of Nanostructured CdSe-Cu ₂ Se Thin Films Moving from Pb to Pb- Free Piezoceramics: A Review Design principles for materials with extreme	78 79 80 81 82 83 84 85 86 87
Mainak Ghosal Jyoti Dutta, Sourav Saikia, Sayeed Ashique Ahmed, Puspendu K. Das Jyoti Sharma, Monika Shukla, Subhasha Nigam, Monika Joshi Krishnaprabha Mapala D. Saritha, R. Sujithra Jyoti Katyal Dr. Sajid Babu Nalakatha, Dr. M. Abdul Khadar Pranati Purohit S C Rakesh Roshan, N Yedukondalu, R Rakesh	2023/FIT/SIT/252 ICRTMD- 2023/FIT/SIT/253 ICRTMD- 2023/FIT/SIT/255 ICRTMD- 2023/FIT/SIT/258 ICRTMD- 2023/FIT/SIT/259 ICRTMD- 2023/FIT/SIT/262 ICRTMD- 2023/FIT/SIT/263 ICRTMD- 2023/FIT/SIT/266 ICRTMD- 2023/FIT/SIT/269 ICRTMD- 2023/FIT/SIT/272	By minosis of Hydrogen Autocomposites by Radiation Assistance for Biomedical Applications Behaviour of Cementitious Systems on Additions of Nano Silica Influence of size and composition on fluorescence properties of carbonaceous nanoparticles (CNPs) Ecofriendly and sustainiable nanomaterials for the removal of hazardous contaminants from wastewater Synthesis of Silver and Gold Nanoparticles using Syzygium samarangense Fruit Extract as Reducing Agent Advancements in Electrode Materials for Lithium-Ion Batteries: A Comprehensive Study Magnetoplasmon Core shell Nanostructure Band-gap Engineering of Nanostructured CdSe-Cu ₂ Se Thin Films Moving from Pb to Pb- Free Piezoceramics: A Review Design principles for materials with extreme Lattice Thermal Conductivity	78 79 80 81 82 83 84 85 86 87

Kumar			
R. Parimaladevi	ICRTMD-	Detection and Degradation of Pharmaceutical	88
	2023/FIT/SIT/274	waste using Bismuth Sulphide Nanoparticles	
		incorporated reduced graphene oxide/Silver	
		substrate	
Jyothilekshmi Indiramma,	ICRTMD-	Synthesis, characterization and biocompatability	89
Kishore K. R. Tetala,	2023/FIT/SIT/275	of macroporous polyhydroxyethylmethacrylate	
Jayaprakash N.S.		based cryogel	
Vikas Kashyap, Sushil	ICRTMD-	Structural analysis of Ag nanoparticles	90
Kumar, Isha, Neeru	2023/FIT/SIT/276	deposited on Si wafer and their influence on Si	
Chaudhary, Navdeep Goyal		nanowire-based Gas Sensor	
Suvankar Chakraborty	ICRTMD-	Tin oxide thin films on $Ag(111)$: thickness and	91
	2023/FIT/SIT/278	temperature dependent study	
Chhavi Sharma, Puneet	ICRTMD-	Bacterial Nanocellulose in Synergy with Herbal	92
Pathak	2023/FIT/SIT/280	Extracts: Production and Characterization	
Samit Kumar, Sundaram	ICRTMD-	Studies on preparation and physico-chemical	93
Khare, Dinesh Kumar Mishra	2023/FIT/SIT/281	characterization of green hydrogels	
Gayatri Patel	ICRTMD-	Revolutionizing Therapeutics: Challenges and	94
	2023/FIT/SIT/282	Innovative Solutions in 3D Printing	
Muralasetti Nookaraju,	ICRTMD-	Synthesis, Electrochemical and Antimicrobial	95
Prakash Gadepalli, Vaddadi	2023/FIT/SIT/283	Studies of Ni(II) Complexes with New Macro	
Krishna		Cyclic Schiff Base Ligands	
Lipsa Nanda	ICRTMD-	Exact Solution of Optical Pulses in Nonlinear	96
	2023/FIT/SIT/284	Meta-materials	
Dr. Nandkishor B. Shirsath,	ICRTMD-	Synthesis of Silver Nanoparticles using	97
Dr. T. S. Savale	2023/FIT/SIT/286	Plumeria plant and its Larvicidal Activity	
		against Malaria Vectors	
H. S. Mund	ICRTMD-	Magnetic Characteristics of $La_{0.7}Ca_{0.3}MnO_3$:	98
	2023/FIT/SIT/288	Insights into the effects of Ni and Co doping	
		through magnetic Compton spectroscopy	
Konica Sharma, M. K. Malik	ICRTMD-	Recent progress in applications of	99
M. S. Goyat	2023/FIT/SIT/289	superhydrophobic coatings and surfaces in	
		various fields	100
Pankaj Chamoli	ICRTMD-	Anisotropic nanostructure hybrids for the	100
	2023/FIT/SIT/292	removal of organic contaminants	101
Amit Rajput, Anuj Kumar	ICRTMD-	Low-Spin Iron(III) Complexes in Neutral,	101
Sharma, Suman K. Barman,	2023/F11/S11/294	Monocation, and Monoanion Forms Stabilized	
Debasis Koley, Markus		by Azo-Appended Iridentate o	
Steinert, Kabindranath		Annuophenoiate (2^{-}) and 0-	
Mukilei jee	ICDTMD	A dyapand Characterization Techniques in	102
Animuddha Mandal Amit	1CKTMD- 2022/EIT/SIT/205	Advanced Characterization Techniques In	102
Kumar Kundu, Dilin K	2025/F11/511/295	Nanocarbon Materials. An inclusive Review	
Maiti Praseniit Mandal			
Revethy C Sunitha V R	ICRTMD-	Lithium Ion Transport Studies in PEO - PMMA	103
Benson K Money	2023/FIT/SIT/299	Based Blend Polymer Electrolyte Systems	105
Radhakrishnan S	2023/11/011/2//	Bused Biend Forymer Electroryte Systems	
Savantan Guha	ICRTMD-	Natures of reflected waves generated due to	104
Sujunun Sunu	2023/FIT/SIT/300	incident aP/aSV waves at the stress-free surface	101
		of a micro-mechanically modeled PFRC half-	
		space	
Neeraj Kumari	ICRTMD-	A Novel Approach for the Synthesis of Nano	105
5	2023/FIT/SIT/304	Pigments and Their Application in Polymer	
		Matrix	
Dr. Krishna Vaddadi	ICRTMD-	Synthesis, Characterisation and Biological	106
	2023/FIT/SIT/306	Activity Studies of Novel Series of Isomeric	
		Pyridyl-Tetrazole Ligands and Bivalent Metal	
		Complexes	
Vinay Kumar, Kalpana R	ICRTMD-	Wound healing and regeneration properties of	107
	2023/FIT/SIT/307	novel biocompatible chitosan biopolymer	
		scaffold	
S. Dey Sadhu, P. Jain, S. K.	ICRTMD-	Preparation and characterization of NBR based	108

Jha, S. Sahoo	2023/FIT/SIT/308	composite of Polythiophene and Modified	
Maintan I. Mittal Hittan Kanada	ICDTMD	Carbon Black	100
Ghosh	1CR1MD- 2023/FIT/SIT/310	from microalgae using nanocatalytic	109
Ghosh	2023/11/311/310	transesterification process	
Dr. Prakash Gadipelli, Dr. Muralasetti Nookaraju	ICRTMD- 2023/FIT/SIT/314	Synergies of Synthesis: Recent Advances and Broader Significance in Chemistry	110
Ruma Das, P. K. Giri	ICRTMD-	Sensing of Fe ³⁺ ions with Nitrogen-doped	111
	2023/FIT/SIT/325	Graphene Quantum Dots functionalized with Au Nanoparticles through Photodetection Method	
Barnali Ghosh (Saha)	ICRTMD-	Low power Paper electronics based Wearable	112
	2023/FIT/SIT/329	Radiation detector by Engineering Perovskite Halides	
Shivananda C S, Sangappa Y	ICRTMD-	Size Modification of Green Synthesized Silver	113
	2023/FIT/SIT/331	Nanoparticles under UV exposure and Its Bacterial Resistance	
Sandip S. Pathade, Bapu S.	ICRTMD-	Synthesis, Characterization and Computational	114
Jagdale	2023/FIT/SIT/333	Investigation of 4-(4-bromophenyl)-2-(4-	
		chlorophenyl)-2,3-dihydro-1H-benzo[b] [1,4]	
Mukash Kumari	ICPTMD	Synthesis and Characterization of	115
Wukesh Kuman	2023/FIT/SIT/338	Superparamagnetic NFO Nanoparticles using	115
	2023/11/01/050	Hydrothermal Method	
Medha Mili, Anju	ICRTMD-	Designing of Flexible and Moldable Bamboo	116
Harsh Bainai Prasanth Nair	2023/F11/511/559	Composites for Thermal Insulation Applications	
A.K. Srivastava, Sarika		Composites for Therman Insulation Applications	
Verma			
Neena P	ICRTMD-	Mechanical study of Polymer composite	117
	2023/FIT/SIT/342	reinforced with surface-modified Napier grass	
Cotore Dol Circola Analysis	ICDTMD	stem cellulose nanofibrils	110
Satya Pai Singh, Archana Kumari Singh	2023/FIT/SIT/350	formed by Selfassembled MgO and ZnO	118
Kuman Singh	2023/11/311/350	Quantum Dots in Presence of LC Media	
Nithyaa N, Muralidharan M,	ICRTMD-	Investigation on SnO2/graphene-based	119
Namagal S	2023/FIT/SIT/352	nanocomposites for supercapacitor application	
Somnath Chowdhury, Tuya	ICRTMD-	Unveiling the potential of two-dimensional V_2S_2	120
Dey, Sung Gu Kang, Jagadish Chandra Mahata, Bikash C	2023/FI1/SI1/353	monolayer as a high-performance anode	
Gupta		principles study	
S.K. Nath, P.K. Kalita	ICRTMD-	Structural, Optical and Ionic conductivity Study	121
	2023/FIT/SIT/354	of Copper Sulphide Quantum Dot Synthesized	
		in Starch Matrix for Its Optoelectronic Device	
D . D .		Applications	100
Pooja Rani	2023/FIT/SIT/358	Graphene the Wonder Material of 21st Century	122
Rajni Bala	ICRTMD-	Design and fabrication of 2D photonic crystals 1	123
Viene Verseeri	2023/FIT/SIT/362	employing electron beam lithography	104
Vinay Kumari	2023/FIT/SIT/364	Thin Films for Advanced Optical Limiting	124
Deathers Ch		Applications	105
Raghav Sharma	ICRTMD- 2023/FIT/SIT/365	Next generation high-frequency rectifiers using	125
Surila	ICRTMD-	A paradox of pollution and purity of Ganga	126
	2023/FIT/SIT/369	River in India	
Aman Dahiya	ICRTMD-2023/ FIT/SIT /370	Systematic Study on Material Selection	127
Anjali Sharma	ICRTMD- 2023/FIT/SIT/372	In ₂ Se ₃ and Bi ₂ Te ₃ thin films based efficient	128
Arijit Chowdhuri	ICRTMD-	Highly efficient low temperature operated NO ₂	129
	2023/FIT/SIT/373	gas sensors	
Gaurav Bajpai, Anuradha	ICRTMD-	Development of Metal Matrix Composites by	130

Bajpai, Rajesh Purohit	2023/FIT/SIT/375	Powder Metallurgy using Cold Isostatic	
		Compaction Chamber: A Review	
Kirandish Kaur, Anita Rani,	ICRTMD-	Structural Stability and Ferromagnetism in	131
Suresh Sharma	2023/FIT/SIT/376	$Ga_{0.875}Cr_{0.125}P$: DFT Study	
Aruna Priya P, Lakshmi	ICRTMD-	Silver Coated 1D Random Photonic Crystals for	132
Thara R	2023/FIT/SIT/379	Sensing of Cancer Cell	
Subhankar Das	ICRTMD-	Assessing the Fracture Toughness and Dynamic	133
	2023/FIT/SIT/382	Crack Propagation behavior of Epoxy	
		Composites Reinforced with Chopped Carbon	
		Fibers	
Manjeet Singh	ICRTMD-	Nonlinear absorption coefficient and refractive	134
	2023/FIT/SIT/383	index of scattered Stokes mode in n-type doped	
		gallium arsenide	

Faculty/ Scientist Talks

Ketan Jagtap, Raju Pawade	ICRTMD-	Impact of Machining Environment on Surface	135
	2023/FT/ST /119	Integrity of Co-Cr-Mo Biomaterial in CNC	
		Precision Turning	
Sibasish Dutta	ICRTMD-	Design and Development of a Smartphone	136
	2023/FT/ST /146	Spectrometer in Visible Domain	
Preetha K C, Bini S	ICRTMD-	Preparation of CuZnS thin films by Chemical	137
	2023/FT/ST /148	bath deposition method and its Characterizations	
Kavitha M V, Anjali C K,	ICRTMD-	Device simulation and optimization of HTL-free	138
Sudheer Sebastian K	2023/FT/ST /149	Perovskite solar cell with CH ₃ NH ₃ SnBr ₃ as the	
		absorber layer by SCAPS -1D software	
Shikha Bathla, Diya Dawar,	ICRTMD-	Design and analysis of SiGe source based Gate	139
Tanu Singh, Pradeep Kumar,	2023/F1/ST /158	All Around core shell dopingless nanotube	
Leo Raj Solay		Tunnel FET	
Vinod D. Deotale, Madhukar	ICRTMD-	UV-Visible Absorption Technique for	140
G. Dhonde	2023/F1/ST /160	Determination of Rate of Synthesis of	
		Thiobarbituric Acids and their Knovenagel	
		Derivatives	
Thamaraiselvi C, S.T. Athira,	ICRTMD-	Green polysaccharide material for the removal	141
P. Elsybai Sweety	2023/F1/ST /162	of colour, TDS, COD and chloride from Dyeing	
		effluent	1.10
Aartee Sharma, Manvendra	ICRTMD-	Tuning Surface Plasmon Resonance of Gold	142
Kumar ² , Parasmani Rajput	2023/F1/S1 /185	using Rippled Si Surface	1.10
Navdeep Sharma, Madan Lal	ICRTMD-	Electrical Charge Transport Exploration 1 of	143
	2023/F1/ST /193	CSA-doped poly (o- methylaniline); A	
		Conducting Polymer	
Shailja Tiwari	ICRTMD-	Growth and properties of metallic and insulating	144
	2023/F1/ST /210	molybdenum oxide thin films	1.1.7
J.H. Markna, Sandhya Dodia,	ICRTMD-	Enhancing Durability and Water Repellency of	145
Gaurav Jadav,	2023/F1/S1 /229	Cement Blocks through Nanostructured S_1O_2	
Pradhumansinh Kher, Tanvi		Coating	
Dudharejiya, Mayur Vala,			
Pankaj Solanki, Hitesh			
Asnani, Bharat Kataria			140
B. Roshan, B. Ravi Teja, U.	ICRIMD-	Effect of Reinforced Particulates on mechanical	146
Krishna Prasad, K. Sanith, R.	2023/F1/S1 /244	properties of AA5059 Based Metal Matrix	
Venkateswara Rao, Prof.		Composite	
1.V.S.S.V. Prasada Rao			1.47
Palvinder Kaur	ICRIMD- 2022/ET/ST /245	Magnetism in semiconductor nanomaterials (A	147
Calle Damana Valamili Cal	2023/F1/S1 /243	Emparative study)	140
Gudia Kamana, Yadavalli Sal	1CK I MD- 2022/ET/0T /257	Experimental Analysis of Metal Matrix	148
Supraja, Tejavath Kajashekar,	2023/F1/81/25/	Composite on ALOUOI/SIC/B4C/Fly-Ash	
Adapatity Kanul, Banothu			
Devender, Prof. 1 v 555 V			
C Succession D. Decare	ICDTMD	Non-coelluloop Summerted Compan Ferrits	140
G. Sreekala, B. Beena	ICKIMD-	Nanocenulose Supported Copper Ferrite	149

	2023/FT/ST /298	Nanoparticles: Synthesis from Simarouba glouca	
Anita Verma Ravi Sharma	ICRTMD-	Synthesis and Photoluminescence Properties of	150
D P Risen Nameeta Brahme	2023/FT/ST /300	Trivalent Bare Earth Doped MgV Al. SiO.	150
Kanchan Tiwari	2023/11/31/307	Phosphor	
Navanand B. Wadwale	ICRTMD-	Experimental and computational investigation of	151
Navanand D. Wadwale	2023/FT/ST /312	Imino-5-methylsulpanyl-1 7-dihydro-[1 2 4]	151
	2020/11/01/012	triazolo[1,5-a] pyrimidine-6-carbonitrile	
Soni Sharma, Jagat Pal Singh	ICRTMD-	Development of Size and Shape dependent	152
Som Shurma, sugar i u Shigh	2023/FT/ST /316	model for vibrational frequency of nanaocrystals	152
Rajasekaran Saminathan	ICRTMD-	Role of artificial intelligence (AI) and machine	153
Abdulla Yahya Ali Nashali	2023/FT/ST /330	learning (ML) in the corrosion monitoring	155
Abdulrahman Ahmed Ali	2023/11/01/330	processes	
Hagawi Shanmugasundaram		processes	
Marappan, N. Shanmuga			
Priva, Farah Shakeel			
	Stud	ent Talks	
Surender, Chandra Mohan,	ICRTMD-	Novel Modification of Activated Charcoal Sheet	154
Rakesh Kumar	2023/ST/105	with Polypyrrole and Silver Nanoparticles for	
		Removal of Hexavalent Chromium in Water	
		Treatment Processes	
Nimitha K C, Jiji Abraham,	ICRTMD-	MXene- Polymer Nanocomposites for Energy	155
Titto Varughese	2023/ST/109	Applications	
Peeyush Phogat, Shreya,	ICRTMD-	Co-existing Dual Morphology of Single-Phase	156
Ranjana Jha, Sukhvir Singh	2023/ST/111	Molybdenum Trioxide: Unlocking Enhanced	
		Electron Transfer Characteristics	
Neeraj Dhariwal, Preety	ICRTMD-	Room-Temperature Ethanol Sensor based on	157
Yadav, Manju Kumari, Amit	2023/ST/112	novel $ZnFe_2O_4$ gel	
Sanger, Vinod Kumar, O.P.			
Thakur			
Shreya, Peeyush Phogat,	ICRTMD-	Exploring the Potential of Tin-Doped Barium	158
Ranjana Jha, Sukhvir Singh	2023/ST/113	Hydride for Advanced Optoelectronic and	
		Catalytic Applications	
Shahid Ahmad Shah,	ICRTMD-	Sintering and Its Role in Modifying Magnesium-	159
Hamnesh Mahajan	2023/ST/114	Zinc Spinel Ferrite: An Analysis of Structural,	
		Morphological, and Magnetic Traits	
Ravinder Kundu, Prabhakar	ICRTMD-	Optimizing Solar Panel Efficiency Through	160
Kaushik	2023/ST/115	Active Cooling Techniques: A Comprehensive	
		Research Exploration	
Ravindra Kumar, Gurupad	ICRTMD-	Hydrothermally Synthesized Nickel-Doped	161
Maity, Susanta Singha Roy,	2023/ST/125	FeS ₂ /WS ₂ nanocomposite as Supercapacitor	
Ashish Kumar Keshari		Electrode Materials	
Ruksana Sirach, Pragnesh N	ICRTMD-	Carboxymethyl cellulose/ β -Cyclodextrin/nickel	162
Dave	2023/ST/132	cobaltite-based nanocomposite for the removal	
		of malachite green	
Akanksha Bhatt, Shashank	ICRTMD-	Salt's function in creating brick-shaped	163
Kailkhura, Priyank Purohit	2023/ST/135	nanoparticles based on carrageenan	
Pranav Menon K, G. Pavan	ICRTMD-	Fracture Properties and computational	164
Akhil, Ajmal Ameen S,	2023/ST/138	characterization of cracks in Internal combustion	
Jagadeesha. T		engine crank shaft	
Talib Raza, Prathmesh	ICRTMD-	Creep materials characterisation under high	165
Malavekar, Dr. Jagadeesha T	2023/ST/139	stress and high temperature conditions of	
		AI6061 alloy	
Sanket Dinkar Borle, Manas	ICRTMD-	Light Material Selection and Dynamic Analysis	166
Ajay Pandey, Jagadeesha T	2023/ST/140	of Differential Gerabox for four wheeler	
		automobile	
Arpit Tripathi, Dr.	ICRTMD-	Computational Stability Analysis of Francis	167
Jagadeesha T	2023/ST/141	Turbine Impeller Using Finite Element Method	
Vishvaa J, Muhammed	ICRTMD-	Enhancement of Structural strength and stability	168

Shafeeh, Jagadeesha T	2023/ST/142	Analysis of Trellis Bike Chasis using Finite	
			1(0
Shantanu Kumar Sanu	ICRIMD-	Development of Nano Bio Fertilizer via	169
	2023/\$1/157	Chemical and Biological Synthesis	
Rashi Bhardwaj, Tinku Basu	ICRTMD-	MOF-Engineered Janus Micromotors:	170
	2023/ST/159	Pioneering the Future of Antibiotic Waste	
		Management	
Lipsa Leena Panigrahi,	ICRTMD-	Antimicrobial peptide-functionalized iron oxide	171
Manoranjan Arakha	2023/ST/161	nanocomposite for effective remediation against	
5		microorganisms	
P Shakkaewal, T Sharma, G	ICRTMD-	Design and fabrication of 23x15x11 CNC router	172
Singh R Sharma	2023/ST/163	machine for Milling	
Java Patel B K Pandey Juoti	ICRTMD-	Formulation of an appropriate equation of state	173
Gupto	2022/87/164	to predict the molting temperature of metallic	175
Oupta	2023/31/104	colide	
Kar Naha Valar D.K	ICDTMD	Solids	174
Km Nena Yadav, B.K.	ICRIMD-	Modeling of the thermal conductivity of metal	1/4
Pandey, Jyoti Gupta	2023/81/166	and metal oxide nanofluids with varying	
		concentration	
Hemlata Deolal, Prashant	ICRTMD-	Thermodynamically Simulating Cool Thermal	175
Raturi, Sanjeev Kimothi,	2023/ST/168	Energy Storage System (CTESS) with	
Sameer Rawat		Encapsulation of Phase Change Material (PCM)	
Tanmay Medhekar, Rajendra	ICRTMD-	Finite Element Analysis of CFRP Composite	176
Kumar Gupta, Sunil Nimje	2023/ST/169	Laminates with Ply-Discontinuities	
Shristi Mishra, B.K. Pandey.	ICRTMD-	Unified model for the studies of band gap of	177
Ratan Lal Jaiswal Ivoti	2023/ST/170	nanosolids with their varying shape and size	
Gunta	2023/01/1/0	hanosonas with then varying shape and size	
Karan Hadwani Tinku Basu	ICRTMD-	Biocompatible and Targeted Nanocomposites	178
Karan Hadwani, Tinku Dasu	2023/ST/172	for Enhanced Magnetic Pesonance Imaging	170
	2023/31/172	Applications: A Comparison Synthesis and	
		Applications: A Comprehensive Synthesis and	
		Characterization Approach	170
T. Suma Chanu, K.	ICRTMD-	Investigation on the optical, dielectric properties	179
Jugeshwar Singh, K. Nomita	2023/ST/173	and AC conductivity of PVA/PVP/ZnO blend	
Devi		based polymer nanocomposites for	
		optoelectronic and electronic device applications	
Preety Yadav, Neeraj	ICRTMD-	Enhanced degradation of Congo-red dye by La ³⁺	180
Dhariwal, Manju Kumari,	2023/ST/175	doped Fe ₂ O ₃ nanoparticles under sunlight	
Vinod Kumar, O.P. Thakur			
Anita Singh, Ekta, Manisha	ICRTMD-	Preparation of Ficus religiosa leaves extract and	181
	2023/ST/177	its applications in green synthesis of zinc oxide	
		nanoparticles and antimicrobial activity	
R.S. Bemina, T. Joselin	ICRTMD-	Structural, Electronic and RDG Analysis on	182
Beaula	2023/ST/180	Cadmium Chloride Adipic Acid by DFT	
		Approach	
Reena Pathak B K Pandey	ICRTMD-	Study of Thermal Expansion Coefficient of	183
Ivoti Gupta	2023/ST/182	Nanomaterials using different equation of state	105
syou oupta	2023/31/102	with varying Shape and Size	
Davi Kuman Daamu Ashali	ICDTMD	Sumthesis and Characterization of	104
Kavi Kullai, Keellu, Asliok	1CK I WID-	Mul 57 0 5E-204 minut family	104
Kumar	2023/51/191	MINU.5Zh0.5Fe2O4 mixed ferrite	
		nanocomposites with CN1	105
Monika, Babankumar S.	ICRTMD-	Applications of the platinum nanoparticle for	185
Bansod	2023/ST/192	Sensitively and Selectively Determination of	
		lead ions using square wave Voltammetry	
R. Deepa, K.A.	ICRTMD-	An Outstanding electrochemical behavior of	186
Vijayalakshmi, K.T.	2023/ST/194	plasma exposed activated carbon derived cotton	
Maheswari		stalk	
Neetu Malik, Neeraj Kumari,	ICRTMD-	Study of Zone Center Phonons in Double	187
Ruby Jindal	2023/ST/195	Perovskite Oxides	
Vaishali Rana. Raniita Ghosh	ICRTMD-	Probing external factors in Advanced Glycation	188
Moulick	2023/ST/197	Endproducts driven metal nanoparticle synthesis	
		for development of a sensing system	
Preeti Meena Bhandari	ICRTMD-	Investigation of adsorption efficiencies of	189
Neerai Kumari	2023/ST/108	graphene oxide and graphene oxide	107
i i i i i i i i i i i i i i i i i i i	2022/01/170	Braphene on de and graphene on de	1

		Montmorillonite composite for the removal of	
		organic dye	
Pradeep Gupta, Jyoti Prakash	ICRTMD-	Polymer Nanohybrid as Efficient Heat	190
Singh, Jyoti Srivastava,	2023/ST/199	Dissipation Material for Effective Cooling	
Mayank Dwivedi		Applications	
Mr. Manjeet Singh, Dr.	ICRTMD-	Unraveling the Cosmos: A Comprehensive	191
Manoj Malik, Dr. Konica	2023/ST/201	Study of General Relativity and its Profound	
Sharma		Implications	
Bhavna Rohilla, Aryan	ICRTMD-	Synthesis, Characterization and Application of	192
Boora, Surender Duhan	2023/ST/207	GdMnFe ₂ O ₄ as an Advanced Humidity Sensor	
Sabina Yesmin, Sk Jahir	ICRTMD-	Multifunctional Polymer supported Bimetallic	193
Abbas, Shyue-Chu Ke	2023/ST/214	Catalyst towards CO ₂ Utilisation, Organic	
		Synthesis and Environmental Aspects	
Anandhakumar Renuka,	ICRTMD-	Nanoencapsulation of Cymbopogon nardus	194
Vallavan Rajkumar,	2023/ST/219	essential oil and their bioactive constituents: A	
kavumkunnel Rasack Sajinu,		novel strategy to control mycotoxin	
kalichamy Sasikala,		contamination in the food system	
Chinnappan Gunasekaran			
Dharmendra Sharma,	ICRTMD-	Study of Thermal Conductivity of Metallic	195
B.K.Pande, Jyoti Gupta	2023/ST/224	Nanoparticles varing shape and size	
Ritesh Yadav, Somvir Arya	ICRTMD-	Coordination Between Recyclers and Pollution	196
	2023/ST/234	Control Board	
Anjika Rani, Deepa Sharma,	ICRTMD-	Animation & Cartoons as learning tools in	197
Sanjay, Suresh Duggal	2023/ST/238	Physics: A perspective	
Umesh Parmar, Dr. Raj	ICRTMD-	Bandwidth Enhancement of Microstrip Array	198
Kumar Verma	2023/ST/239	Antenna using Gap Coupled Parasitic Patches	
Ravi Sankar Reddy M, S	ICRTMD-	Effect of Fe dopant on ZnS nanoparticles	199
Kaleemulla	2023/ST/242	synthesized from solid-state reaction	
Himani Chaudhary, Peeyush	ICRTMD-	Morphological and Optical Studies of	200
Phogat, Shreya, Ranjana Jha,	2023/ST/247	Hydrothermally Synthesized NiO/NiS	
Sukhvir Singh		Nanocomposite	
Tamanna Jindal, Peeyush	ICRTMD-	Morphological and Optical Analysis of	201
Phogat, Shreya, Ranjana Jha,	2023/ST/248	Tungsten Oxide Nanosheets for Gas Sensing	
Sukhvir Singh		Application	
Sumant Saurav, Satyam Saroj	ICRTMD-	Numerical Modelling and Simulation of Phase	202
, Jagdeesha T	2023/ST/251	change material Melting	
Sanjeet Grewal, Peeyush	ICRTMD-	CTAB-Assisted Hydrothermal Synthesis of	203
Phogat, Shreya, Ranjana Jha,	2023/ST/256	MoO ₃ Nanoparticles: Multifaceted	
Sukhvir Singh		Characterization and Analysis	
Vijay Yadav, Dr. Pramod	ICRTMD-	Fabrication and Characterization of Perovskite	204
Kumar	2023/ST/267	Oxides: Insights into Structural and Functional	
		Properties	
Kuldeep T. Padhyar, Dr. R.S.	ICRTMD-	Synthesis, Characterisation and Computational	205
Nirwan	2023/ST/270	study of Meldrum acid Chalcone Derivatives by	
		using green base	
Shikha Yadav, Shreya,	ICRTMD-	Hydrothermal Synthesis and Characterization of	206
Peeyush Phogat, Ranjana Jha,	2023/ST/273	Tin Telluride	
Sukhvir Singh			
Vinay Rawat, Pankaj	ICRTMD-	Activated Charcoal for the Elimination of	207
Chamoli	2023/ST/285	Methylene Blue Dye from Aqueous	
Vigneshkumar Devaraj,	ICRTMD-	Valorisation of Sand Hydrocyclone Washing	208
Jeevanantham Murugasamy,	2023/ST/287	Wastes (SHWW) as Flowable Fills for	
Gayathri Bairaraju, Sneka		Sustainable Construction Practices	
Murugan, Jeevanantham			
Venkatesh, Soundara Balu,			
Vasudevan Mangottri			
A Jayaraman, M Vasudevan,	ICRTMD-	Design Aspects of Lightweight Building Blocks	209
S Sowsuriya	2023/ST/290	using a Novel Mixture of Nanomaterials for	
		Low-Cost Construction	
A Jayaraman, S	ICRTMD-	A Comprehensive Structural Design-based	210
Parthasarathy, S Vignesh, M	2023/ST/291	Protocol for Energy-Efficient Buildings for	
Vasudevan		Smart City Projects	

Garima, B.L. Choudhary	ICRTMD- 2023/ST/293	Tuning the Structural and Dielectric Properties of ZnFe ₂ O ₄ through Varied Annealing Temperatures	211
Chaithra R, Renuka C.G.	ICRTMD- 2023/ST/296	Investigation and Comparison of the Optoelectronic Properties of Natural Dyes Derived From Methanol and Aqueous Extract of Argyria cuneate Flower	212
Sapna, Chhavi Sharma, Puneet Pathak	ICRTMD- 2023/ST/297	Nano-Innovations in Post-Harvest Preservation: A Holistic Approach to Fruits and Vegetables	213
Vanshika Gairola, Pankaj Chamoli	ICRTMD- 2023/ST/301	Activation of charcoal at low temperature for	214
Harshitha D., Renuka C.G.	ICRTMD-	Natural Dyes To Light Harvesting Materials: A	215
	2023/ST/303	Study On Optoelectronic Properties Of Carissa Carandas Fruits	
Akhilesh K. Yadav, H. Tripathi, S. Rajput, P. Singh, Ashutosh K. Dubey, Krishan Kumar, R. Chawla, Chandana Rath	ICRTMD- 2023/ST/305	Drug kinetics and antimicrobial properties of quaternary bioactive glasses 81S(81SiO ₂ -(16- x)CaO-2P ₂ O ₅ -1Na ₂ O-xMgO); an in-vitro study	216
Afsana Khatoon, Shaziya Siddiqui	ICRTMD- 2023/ST/313	Efficient Removal of Diclofenac Sodium using Cellulose-Based Luffa Actangula Peel Adsorbent: A Promising Approach for Water Treatment	217
K. Mohammed Salman, Mohamed Zikriya, C.G. Renuka	ICRTMD- 2023/ST/315	Band gap enhancement in Mg-Doped ZnO Thin films by sol-gel spin coating method for optoelectronic applications	218
Ismail Sk, Nandan Pakhira	ICRTMD- 2023/ST/317	Exploring the Impact of Strong Correlation and Spin-Orbit Coupling Effects in LuB ₄ : A First- Principles Study	219
Chandra Shekhar Verma, Neelam Shukla, Purna Bose	ICRTMD- 2023/ST/318	Study of Surface Morphology & Elemental investigation of Chemically Deposited Mixed Based (Cdx-Pby-Znz)S Films	220
Anshika Dubey, B.K. Pandey, Priyanshu Srivasatva	ICRTMD- 2023/ST/319	Study on the structural and electrical properties of Solid Oxide Fuel Cell (LaGaO ₃)	221
Bhupali Deka, Dhanjit Talukdar, D. Mohanta	ICRTMD- 2023/ST/320	Experimental and theoretical investigation into the effect of low energy C^{2+} ion irradiation on few layer WS ₂	222
Poonam Rani, Rita Dahiya, Sunil Kumar, Mamta Bulla, Vinay Kumar	ICRTMD- 2023/ST/321	Thermal-Driven Formation of Reduced Graphene Oxide Nanosheets: A Novel Approach to Superior Supercapacitor Electrodes	223
Mini Yadav, Sandeep Yadav, Ajay Shankar, Renu Bala, Mamta Rani	ICRTMD- 2023/ST/322	Effect of Thickness on Structural, Morphological and Optical Properties of thermally evaporated Nichrome thin film	224
Anil Malpotra, Beant Singh, Lakhvir Singh	ICRTMD- 2023/ST/323	Effect of Various Input Process Parameters on Surface Finishing and Materaial Removal Rate in Electrolytic Magnetic Abrasive Finishing	225
Dhanjit Talukdar, Gazi Ameen Ahmed	ICRTMD- 2023/ST/324	Investigation of structural, electronic, and optical properties of Li doped hexagonal boron nitride monolayer through Green's function	226
Manish Kumar Manjhi, Abhishek Pathak, Chandrama Prakash Upadhyaya	ICRTMD- 2023/ST/326	Encapsulation of Bioactive Organosulfur Compounds in Solid Lipid Nanoparticles to Combat Multi Drug Resistance Pathogen	227
Kudzai Hamish Ruzvidzo, Manish Jain, Raminder Kaur	ICRTMD- 2023/ST/328	Rheological, Physical, Thermal, Spectroscopical, Chemical and Electrical properties of novel organic draw solutes for forward osmosis desalination of brackish and seawater feed solutions	228
Ayush Chaurasia, Km. Khushboo Singh, Satya Pal Singh, Archana Kumari Singh	ICRTMD- 2023/ST/332	Preparation and Characterization of Self- Cleaning Hydrophobic Surfaces Using n(ZnO)Coated Glass	229
Himanshi Chauhan,	ICRTMD-	Green Synthesis of Magnesium Oxide NPs	230

	2022/05/224		
Himanshi Yadav, Satya Pal	2023/81/334	Using Chea Seeds and Investigation of Their Antibacterial Effect	
Anil Pakeba Sudam Chayban	ICPTMD	Tailoring optoalectropic properties of	221
Ann Kaksne, Sudan Chavnan	2023/ST/335	hydrothermally synthesized Sn doped nickel	231
	2025/51/555	oxide thin films	
Ayush Yaday, Satya Pal	ICRTMD-	Synthesis of Nano-crystalline Thin	232
Singh Archana Kumari	2023/ST/336	Ferromagnetic Films and Investigation of Their	252
Singh	2020/01/000	Thickness Dependent Magnetic Properties	
Milind C. Nagare	ICRTMD-	Synthesis of silver Nanoparticles used in tridax	233
	2023/ST/337	procumbens leaf extract and their	
		characterization	
Himanshi Yadav, Himanshi	ICRTMD-	Synthesis of Carbon Nanodots via Green Routes	234
Chauhan, Satya Pal Singh,	2023/ST/343	and Investigation of Their Antiviral Effect	
Amar Preet Kaur, Vivek			
Hada			
Anjali Kumari, Savita Soni,	ICRTMD-	M ^{II} [Zn/Mg/Ni]Al-NO ₃ /Cl Layered Double	235
Ajay Sharma, Anil Kumar	2023/ST/344	Hydroxide as Electrode Material for Dye	
Sharma		Sensitized Solar Cell Application	
Divya Venu, Ayushi Jaiswal,	ICRTMD-	Green Synthesis And Characterization Of Cow	236
Kajal Yadav, A.K.	2023/ST/345	Dung/Bamboo Fibre Derived Polyaniline-Based	
Srivastava, Sarika Verma		Composite for Energy Application	
Naved Siraj, S.A.R. Hashmi,	ICRTMD-	Investigating the Thermal and Mechanical	237
Sarika Verma	2023/\$1/346	Synergy of PEEK/GNP Nanocomposites	020
Kajal Yadav, Kamana	ICR I MD-	Robust Synthesis and Antimicrobial	238
Chaturvedi, Anju Singhwane,	2023/51/348	Applications of Bismuth Oxide/ Graphene	
Avallish Kullar Shvastava, Sarika Verma		Nanocomposite as Biomedical Material	
Awantika Shahi Satya Pal	ICRTMD-	Size Dependent Estimation of Bandgaps: From	239
Singh Manish Mishra	2023/ST/349	Synthesis to Formulation	237
Shweta Agrahari	2020/01/01/0	Synthesis to Formulation	
Md Imran, Manish Dhangar.	ICRTMD-	Synthesis And Study Of Thermal Insulating	240
Chandra Shekhar Nayak,	2023/ST/356	Characteristics Of Bio Sludge / Fly Ash-Based	
Raju Khan, Sarika Verma		Geopolymer Binder Composite Material For a	
		Sustainable And Constructive Approach	
Vijayendra Kumar Tripathi,	ICRTMD-	Photocatalytic Reaction Chemistry of	241
Manish Shrivastava, Raju	2023/ST/359	Sustainable Graphene Aerogel for Sequestration	
Kumar Gupta, Jaya Dwivedi		of Pharmaceutical Residues	
Sriparna Paul, Harsh Bajpai,	ICRTMD-	Study of Effort of Temperature and Binder on	242
Medha Milli, Sarika Verma	2023/ST/366	Brine Sludge Based Composite Material	
Dr. Nimish Shah, Uchitesh	ICRTMD-	Innovative Approach to Achieving Zero Liquid	243
Shettyan, Heli Modi, Avadhi	2023/ST/367	Discharge in the Dye Intermediate Sector	
Jain, Arya Yadav			
Akash Ahlawat, Ashish	ICRTMD-	A Neural Network Approach to Enhance FDM	244
Phogat, Watan Pal, Shivam	2023/81/368	3D Printing Parameters for PEIG: Optimizing	
Sabday, Daapaly Chhabra		with Validation Using MOCA ANN	
Ramesh Kumar Garg		with validation Using MOGA-ANN	
Unender Punia			
B Mamatha N Pradeen V	ICRTMD-	Nano Wear Circuits: Multiwalled Carbon	245
Uma, S. Mahendra Kumar	2023/ST/380	Nanotubes Transforming Yarn into Strain	273
Cina, S. Manendra Rumai		Sensors	
Neetu Kumar, Bijov Kumar	ICRTMD-	In today's High-Frequency Environments	246
Kuanr	2023/ST/381	Heterostructured 2D MoS ₂ /Ferrite	
		Nanocomposites Serve as Exceptional	
		Microwave Absorber Material	



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Abstract

The talk will discuss the challenges in developing corrosion resistant graphene coating on most common engineering alloys, such as mild steel, and present recent results demonstrating circumvention of these challenges.

Corrosion and its mitigation costs dearly (any developed economy loses 3-4% of GDP due to corrosion, which translates to ~\$300b to annual loss USA). In spite of traditional approaches of corrosion mitigation (e.g., use of corrosion resistance alloys such as stainless steels and coatings), loss of infrastructure due to corrosion continues to be a vexing problem. So, it is technologically as well as commercially attractive to explore disruptive approaches for durable corrosion resistance. Graphene has triggered unprecedented research excitement for its exceptional characteristics. The most relevant properties of graphene as corrosion resistance barrier are its remarkable chemical inertness, impermeability and toughness, i.e., the requirements of an ideal surface barrier coating for corrosion resistance. However, the extent of corrosion resistance has been found to vary considerably in different studies. The author's group has demonstrated an ultra-thin graphene coating to improve corrosion resistance of copper by two orders of magnitude in an aggressive chloride solution (i.e., similar to seawater). In contrast, other reports suggest the graphene coating to actually enhance corrosion rate of copper, particularly during extended exposures. Authors group has investigated the reasons for such contrast in corrosion resistance due to graphene coating as reported by different researchers. On the basis of the findings, author's group has succeeded in demonstration of durable corrosion resistance as result of development of suitable graphene coating.

Keywords: Graphene; Chemical vapour deposition; Corrosion resistance; Coatings.



Biography: Professor Raman Singh's primary research interests are in the relationship of Nano/microstructure and Environment-assisted degradation and fracture of metallic and composite materials, and Nanotechnology for Advanced Mitigation of such Degradations. He has worked extensively on advanced materials (e.g., graphene) for corrosion mitigation, stress corrosion cracking, and corrosion-mitigation. He is a senior professor at Monash University, Australia. He is/was a Guest Professor at ETH Zurich, Switzerland (2020, 2023, 2024), US Naval Research Lab, Indian Institute of Science, and University of Connecticut. Prof Singh's professional distinctions and recognitions include: Guest Professor of ETH Zurich, Editor of a book on Cracking of Welds (CRC Press), Lead Editor of a book on Non-destructive Evaluation of Corrosion (Wiley), Editor-in-Chief of an

Elsevier and two MDPI journals, leader/chairperson of a few international conferences and numerous plenary/keynote lectures at international conferences, over 265 peer-reviewed international journal publications and 15 book chapter, and several competitive research grants. He has supervised 55 PhD students.

Improved Performance of Rose Bengal Dye-Encapsulated Plasmonic Au Nanoparticlesbased Fiber-Optic Humidity Sensor

S. K. Ghoshal

Physics Department and Ibnu Sina Institute for Scientific and Industrial Research (ISI-SIR), Faculty of Science, Universiti Teknologi Malaysia

Abstract

High performance, reliable and low-cost fiber-optic relative humidity sensors (FO-RHS) with fast response became ever-demanding. Compared to the conventional sensors, the FO-RHS are advantageous due to their simple operation, high stability, and efficient signal detection. Despite the existence of various chemiresistive humidity and gas sensors made of polymers and hybrid inorganic/organic nanomaterials, a high quality RHS with excellent linearity, short response time, and low hysteresis remains deficient. The health-care and food processing sectors worldwide require ultrasensitive materials for RHS fabrication, proposing various compact designs such as side-polished, tapered, and hetero-core fibers. Presently, the functionalized gold nanoparticles (AuNPs)-incorporated fluorescent organic molecules are used as real-time humidity biosensors for respiratory diseases diagnoses. Commercially accessible RHS materials including electrolytes, organic polymers, and ceramics have issues involving sensitivity, reversibility, or medical resistance. Rose Bengal dyes (RBD) being excellent photosensitizers owing to their several notable attributes were utilized for the encapsulation of AuNPs. Thus, the pruned triangular AuNPs (with enhanced fluorescence and LSPR absorption) surface were modified by RBD molecules for more water molecules adsorption and extra charge carriers trapping at the metalsemiconductor Schottky contact thereby improving the RHS response. The synergy between nanosized receptor layers and optical fiber platform was established to provide a strong humidly sensing trait. These stable RBD molecules-decorated AuNPs grown at optimum laser fluence by PLAL method showed better sensitivity and linearity than the one coated with pure AuNPs when tested against polyvinyl alcohol. Strong attachment of -OH and COOH functional groups of RBD onto AuNPs surface was responsible for PVA molecules sensing via the hydrogen bonds formation.



Biography: Sib Krishna Ghoshal (Condensed Matter Physicist) is Professor at Physics Department and Laser Center, Faculty of Science, Universiti Teknologi Malaysia. He received PhD from JNU (Delhi) and was postdoctoral fellow at Brandeis University (USA) and IIT (Delhi) & Oxford University (UK). He published over 685 research articles, 20 book chapters, and 7 books with Google Scholar h-index of 48, i10-index of 170 and citations of 8376. He received 58 research grants, two patents on the proposed anticancer drug formulation and plasmon humidity sensor, supervised 30 PhD, 81 MSc & 63 Undergraduate theses. He is recognized as Top 2% of Scientists in their Field Worldwide in 2019, 2021 and 2022 by Stanford University (USA) rankings.

ICRTMD-2023/KT/003 Ion beams, Lasers and Gamma Radiations in Nano Science and Nano Technology

Anand P Pathak

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Abstract

We have been using swift heavy ion beams, Lasers and Gamma Radiations to synthesize and modify nanostructures of elemental as well as compound semiconductors and subsequently characterizing themusing XRD, Raman and TEM. An overview of the dependence of the resulting new class of nano-materials on energy and fluence of the initial swift heavy ions and Lasers will be presented. These external radiations modify the electronic and optical properties of nano-structures (quantum wells, quantum dots and nanowires). Some applications of these studies in Nanotechnology in general and opto-electronic devices in particular along with their relevance in energy research as well as biosciences, will also be discussed during this Conference on Materials Science & Devices (ICRTMD 2023).



Biography: Prof. Anand P. Pathak received Ph.D. degree from IIT Kanpur in 1971. He has published 317 research papers in reputed International Journals. Currently he is NASI Sr Scientist Platinum Jubilee Fellow (Since 1st Feb 2020 onwards) (& Honorary Professor of Physics Since Oct 2017 onwards at University of Hyderabad). He has been Guest Scientist (at foreign institutions) since joining University of Hyderabad in July 1977 including H.C. Orsted Institute, Copenhagen (Denmark); CSIRO, Division of Chemical Physics, Clayton (Australia); Max Planck Institut fur Metallforschung, Stuttgart (W. Germany); ICTP, Trieste (Italy); Universitat Freiburg, Germany (Humboldt Fellow); Forschung Zentrum Rossendorf (Dresden) Germany (Humboldt Fellow); Universidad Autonoma Metropolitana, Iztapalapa (Mexico City); Visiting ("Alonso Fernandez Gonzalez" Chair) Professor in Physics, one year

Sabbatical Leave from Hyderabad); University of Padova (Italy) (Visiting Professor); Frankfurt Institute for Advanced Study (FIAS) Uni Frankfurt (Humboldt Fellow); Institute for Nuclear Studies and Institute for Electronic Materials Technology Warsaw, Poland and many more...

ICRTMD-2023/KT/004 Oxide nanoparticles reinforced polymer nanocomposites for advanced applications

Manjeet Singh Goyat

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Abstract

Over the past three decades, toughening of epoxy polymers by oxide nanoparticles gained significant attention. The brittle nature of epoxy polymers limits their use in advanced structural applications where safety is a major concern. Rigid spherical oxide nanoparticles offered several advantages over other nanostructures for reinforcing epoxy polymers such as lowtoxicity, non-conductivity, availability, economical, and low aspect ratio (\sim 1) making them easy todisperse in viscus or semi-viscous polymers. The organized dispersion of oxide nanoparticles have an inordinate competence to toughen the epoxy polymers. Functionalized oxide nanoparticlesembedded in polystyrene polymer can be used to develop transparent superhydrophobic coatings for energy industryand corrosion resistant coatings for metal industry. Additionally, the development of shear thickening fluids using oxide nanoparticles is very crucial to develop advanced flexible body armor for the defense industry.

Keywords: OxideNanoparticles, Polymer nanocomposites, Superhydrophobic coatings, Flexible body armor.



Biography: Dr. Manjeet Singh Goyat earned his dual master's degree M.Sc. in Physics and M.Tech. in Nano Science & Technology from Guru Jambheshwar University of Science and Technology, Hisar, India. His journey continued with a PhD in Materials Engineering from the Indian Institute of Technology Roorkee. Presently, he is working as a Visiting Researcher at Smart Materials, Mads Clausen Institute, University of Southern Denmark, Denmark. He holds the position of Senior Associate Professor in the Cluster of Applied Sciences at the University of Petroleum and Energy Studies, Dehradun, India.

His extensive research is dedicated to polymer matrix nanocomposites, selfhealing polymer matrix composites, hybrid polymer nanocomposites,

nanomaterial synthesis and functionalization, process optimization, as well as superhydrophobic coatings for self-cleaning and anti-corrosion applications.

Noteworthy honors include being a recipient of the DST SERB SURE funding and the DST SERB SIRE Fellowship. With a substantial publication record, Dr. Manjeet has authored over 60 research papers in peerreviewed journals and contributed to 6 book chapters for reputed publishers including RSC and Elsevier. He delivered more than 20 scientific talks at national and international conferences. In September 2021, he presented an Invited Scientific Speech at a prestigious Scientific Meeting of The Royal Society.

Dr. Manjeet's involvement in academic and editorial roles is commendable. He served as a Guest Editor for the Frontiers in Materials Journal. Additionally, he holds the position of Editorial Board Member for Materials Protection, a Scopus Indexed Journal by the Engineers Society for Corrosion Republic of Serbia, Belgrade. Notably, he serves as the Editor-in-chief of RP Current Trends in Engineering and Technology Journal, published by Research Plateau Publishers.

His commitment to nurturing academic talent is evident through his supervision of 1 PhD student and ongoing guidance for 8 PhD students. Furthermore, Dr. Manjeet has supervised numerous undergraduate students for their minor and major projects, including facilitating internship projects to 2 French students. He remains an active reviewer for several high-repute peer-reviewed scientific journals and has contributed as a Reviewer for Internal Research Grants of Qatar University, Qatar.

Tetrapods based Smart Materials for Advanced Technologies

Yogendra Kumar Mishra

Professor WSR

Mads Clausen Institute, NanoSYD, Smart Materials University of Southern Denmark, Alsion 2, 6400, Sønderborg, Denmark

Abstract

Considering the size dependent utilization complexities of nanoscopic dimensions towards real applications, the focus of nanomaterials community is merging to three-dimensional (3D) form of materials which are built out of interconnected anisotropic nanostructures. This talk will briefly introduce the importance of tetrapod shaped nanostructures towards smart 3D nanostructuring. A simple flame based single step approach was developed for synthesizing zinc oxide tetrapods which demonstrated many applications in different technologies. These tetrapods have been used as building blocks to construct highly porous interconnected 3D nanonetworks in form of flexible ceramics which offer many new application avenues. Additionally, these smartnanonetworks have been utilized as sacrificial templates to develop hollow tetrapodal 3D networks from almost any desired material (carbons, nitrides, oxides, polymers, hydrogels, etc.). The sacrificial template-based strategy offers new and unique opportunities in the direction of 3D nanomaterials engineering and accordingly advanced technological applications [1-10]. The scopes of 3D nanomaterials engineering will be demonstrated along with their applications [1-10]. The scopes of 3D nanostructuring based smart materials in sensing, electronics, optoelectronics, energy, biomedical, and photonic engineering technologies, etc. will be briefly highlighted in the talk.

Keywords: Smart Materials, Tetrapods, Hybrid Nanomaterials, Advanced Technologies.



Biography: Yogendra Kumar Mishra is Professor MSO at Mads Clausen Institute, NanoSYD, University of Southern Denmark (SDU), Denmark. Prior joining to SDU, he worked as group leader at Kiel University, Germany. He did Habilitation in Materials Science from Kiel University in 2015 and Ph. D. in Physics in 2008 from Jawaharlal Nehru University (Inter University Accelerator Centre), New Delhi, India. In Kiel, he introduced a new flame-based process for metal oxide tetrapod nanostructuring and their 3D networks which showed many applications in engineering and biomedical fields. Additionally, tetrapods can be used as templates to

create hybrid and new 3D materials. At NanoSYD, he is heading 'Smart Materials' group with the focus to develop new materials for green and sustainable technologies. He is Humboldtian and recently honored with FRSC- Fellow of Royal Society of Chemistry.

- Publications > 350, Citations > 17900, H-index: 72
- Editorial Board Member/Associate Editor for several high impact for magazines

https://portal.findresearcher.sdu.dk/en/persons/Mishra https://scholar.google.com/citations?user=TW4Bq_oAAAAJ&hl=en

Mesoporous Materials in Sensing Applications

Surender Duhan^{*}, Bhavna, Supriya Sehrawat, Aryan Boora, Priya, Anisha, Sushma

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Abstract

Porous materials are ubiquitous around the world, and nearly all the earth's solid contents are porous to some extent. The application of clay, wood, and other porous materials do not have any well-documented beginnings, but certainly date back to prehistoric times. These porous solids in the form of natural material or with heat treatment were already used by early humans. Nowadays, the synthesis, characterization, and application of novel porous materials have been strongly encouraged globally due to their wide range of applications in adsorption, separation, catalysis, sensors, drug delivery and environmental pollution control. The design, synthesis, and modification of porous materials are in some aspects more challenging than the synthesis of dense materials. The increasing interest in porous materials is because of their ability to interact with atoms, ions, molecules, and nanoparticles not only at their surfaces, but throughout the bulk of the materials. Therefore, the presence of pores in nanostructured materials greatly promotes their physical and chemical properties. The innovative synthesis strategies, an evolution toward structured materials with larger pores could be obtained. After the first reports that introduced the M41S family of ordered mesoporous silicas at the beginning of the 1990s, the synthesis of advanced mesoporous materials has undergone explosive growth. Recently, the understanding, design and manipulation of pores have significantly advanced science and technology, and have been playing increasingly important roles in modern society.

Keywords: Mesoporous; adsorption; materials.



Biography: Dr. Surender Duhan, an Associate Professor is currently active in his research work and teaching skills in Department of Physics, Deen Bandhu Chhotu Ram University of Science and Technology, Murthal, Sonipat (Haryana). He received his Ph.D. degree from Guru Jambheshwar University of Science & Technology, Hisar in 2009. He leads a research group dedicated to the 'Synthesis and Characterization of functional materials', especially porous metal oxides for applications in humidity sensing, gassensing, photo catalysis, bio active glasses, anti cancer and drug delivery system'. He has completed three major projects with CSIR, MHRD and UGC. He has written more than 125 research papers in reputed International/National Journals and has granted 3 Patents. His publications have more than 3000 citations with *h*-index 29 and *i*-index 52. At present, he is member of Research Promotion Board in DCRUST, Murthal, Sonepat, Haryana (India). He was a member of PGBOS and DRC in Dept. of Materials Science and Nanotechnology from 2010 till date.

ICRTMD-2023/KT/007 NanoBiomaterials for the Therapy of Experimental Inflammatory Arthritis

Rehan Khan

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Abstract

Rheumatoid arthritis (RA) is an autoimmune disorder affecting about 1% of global population and in severe cases, disease may lead to permanent disability. Its pathogenesis implicates synoviocytes hyperproliferation, angiogenesis, formation of pannus, along with cartilage and bone degradation, which causes damage and disability. Besides substantial progresses in treatment standards, some limitations are there still there such as enhanced drug metabolism and high clearance leads to low bioavailability of anti-rheumatic drugs. We have developed a new type of nanomedicine in which we conjugated caffeic acid with polyethylene glycol-polycaprolactone (PEG-PCL) to make it therapeutic nanocarrier by conjugation caffeic acid as caffeic acid has potent anti-arthritis and anti-inflammatory effects and it inhibits NF-kB molecule. Moreover, we have entrapped 9-aminoacridine (9-AA) drug which has been reported to possess anti-inflammatory effects by activating NR4A1 molecule. Therefore, our developed nanomedicine has dual targeting nanoparticles and exhibited significant efficacy against collagen-induced arthritis. The plausible therapeutic action of nanomedicine might be due to the inhibition of NF-kB and NR4A1 molecules.

Keywords: Rheumatoid arthritis; 9-aminoacridine; Caffeic acid; Nanomedicine.



Biography: Dr Rehan Khan is working as a Scientist-D at Institute of Nano Science and Technology (INST), Mohali. Prior to this, he worked as a post-doctoral fellow at the University of Manitoba, Canada. He obtained his PhD from Hamdard University, New Delhi. The research in his laboratory at INST focuses on the design and development of therapeutic nanomicelles or nano-sized delivery systems for the management of experimental rheumatoid arthritis (RA) and Ulcerative colitis The research also focuses on the development of nanoparticles for the synthetic lethal therapy for colorectal cancer. He is also working on the safety assessment of nanoparticles using rat/mice models. He has published more than 90 journal articles such as ACS Nano, Chemical Engineering Journal, Biomacromolecules etc, and 15 book chapters with a total of 3500 citations, with 35 h-index.

Indra Sulania^{1,3*}, Ambuj Tripathi¹, Ranjeet K Karn², Elham Chamanehpour³, Ajani Lakmini Jayarathna^{3,4} and Y K Mishra^{3*}

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Abstract

Environmental remediation is the key concern nowadays due to increasing burden of pollutants in waterbodies. In this study, Zinc oxide tetrapods (ZNT) based polymer compositecatalyst were synthesized with different concentration of ZNT dissolved in Polyethylene Glycol (PEG) solution through chemical routes for the wastewater treatments. Synthesized solution was probe sonicated at 20W and spin coated on glass and CaF₂substrates followed by characteristic analysis using SEM with EDX, FTIR and UV-Vis. spectrophotometers. SEM images confirms the composite formation of ZNT with PEG with their legs intact, thus, forming 3D catalyst electrode. FTIR confirms the presence of functional groups for the synthesized composite samples. Absorbance for PEG and ZnO were observed at lower wavelengths. Further, degradation of methylene blue dye was studied in the presence of the catalyst with UV exposure time and the degradation was found to improve in the presence of composite sample due to efficient charge separation. The (ZNT+PEG) catalyst and found to be promising alternative for wastewater treatment and thus, in environmental remediation.

Keywords: ZnO tetrapods, Photocatalyst, Polymer composite, SEM, FTIR spectroscopy.



Biography: Dr. Indra Sulania has been working as a Scientist at Inter University Accelerator Centre, New Delhi, for nearly 20 years. She has been awarded with a prestigious SIRE fellowship from SERB, DST, Govt. of India. She did her Ph. D. in Physics from Jamia Millia Islamia, Delhi, in 2016. She has more than 100 papers in internationally reputed Journals with more than 1000 citations. She has served as an associate editor for Frontiers in Physics Journal and is a part of reviewer's team for Elsevier, Science Direct, Wiley and Springer and many more publication teams. She has been a part of many organizing committees for national and International Conferences related to ion beams and applications. Her areas of research are Sensors and catalysis, radiation resistant and shielding materials, Ion beam induced modification of surfaces and applications, polymer composites etc. She is incharge of Materials Science experimental beamline in beam hall-1, Scanning Probe Microscope and few major equipment in IUAC, New Delhi.

ICRTMD-2023/KT/009 Miniaturized electron source with low dimensional materials: Emerging applications

Santanu Ghosh

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Abstract

A constant endeveour is in progress to make ultra small electron sources with high intensity and better temporal stability using quantum mechanical tunneling process of electrons.

In this talk field emission (FE) properties of two types of nanostructured composite films, promising novel materials for third generation electron sources and displays: (i) Nanoparticle decorated multi-walled carbon nanotubes (MWCNTs)-and (ii) metal-insulator nanocomposite thin-films will be discussed.

FE measurements were carried out in an indigenously developed high vacuum diode set up. The salient results obtained can be summarized as (i) a significant improvement of FE current and temporal stability associated with an appreciable reduction in turn-on field from metal nanoparticle (Metals, LaB_6 and CeB_6) decorated MWCNT-films as compared to only MWCNT films: showing promises for electron-guns, x-ray sources etc.; (ii) appreciable increase in FE current density with high mechanical durability in metal nanoparticle decorated composites: promising planar emitter for future flat-displays. The enhanced FE characteristics of these emitters are understood from a combined experimental results, electronic structure first-principles based calculations study.



Biography: Santanu Ghosh, Professor, Department of Physics, IIT Delhi has long expertise in the field of Nanocomposites, Carbon nanotubes, Magnetic nanoparticles, Ion materials interaction and field emission of electrons. He worked as PI of 5 international project, which include one prestigious CRP funded by IAEA, UNO. He is also PI of 11 national project. He has delivered ~55 talks, which include invited, keynote address and plenary, published one books, 8 book chapters, 125 papers in peer reviewed journals and created one NPTEL lecture series. He was DST-BMBF fellow in the year 2000, DST-DFG fellow in 2005-2006, DAAD fellow 2010 and 2013 and delegate to IAEA, Viena in 2012 and 2015. He was national cocordinator of PMRF (200-2022), IAAM Medal scientist (2023), member of MRSI, MSI, MRS Singapore (annual member), ACS (annual member) and invited member for review committee of polish science foundation projects (2012-13).

ICRTMD-2023/KT/010

Strategies for Lowering Operation Voltage of Organic Field Effect Transistors

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Abstract

Intensified research efforts have been dedicated to reducing the operational voltage in Organic Field-Effect Transistors (OFETs) due to the increasing demand for energy-efficient and flexible electronic devices. OFETs are crucial for the seamless integration of organic electronics in various applications, including wearable devices and Internet of Things (IoT) sensors. The development and characterization of functional organic materials for use as conducting and insulating layers in electronic devices is a major area of scientific and technological research. The aim is to enable the production of high-performance electronic circuitry on large, flexible substrates at a low cost. Although organic field-effect transistors (OFETs) have been studied extensively over the past few decades as alternatives to conventional silicon-based semiconductor devices, only recently have they exhibited notable characteristics. These include high charge carrier mobilities exceeding 40 cm²/V·s and commendable device stabilities, albeit at relatively elevated operational voltages surpassing 40 V. To achieve optimal performance in low-voltage OFETs, it is necessary to use gate insulators with superior dielectric properties and high compatibility with the organic semiconductor. Additionally, facile, cost-effective, and dependable materials deposition methods are required. Recently, ion-gel electrolytes have gained interest as dielectric materials due to their substantial capacitance and easy integration into OFETs. Poly(methyl methacrylate) (PMMA) has been shown to be a reliable polymer dielectric for stable, high-performance allorganic top-gate/bottom-contact FETs. However, due to its low dielectric constant (k < 3.5), the operating voltages of corresponding OFETs tend to be high (> 40 V), which can be exacerbated by a high density of pinholes.Using plasticized form of polymethyl methacrylate (PMMA) as a gate dielectric emerges as a new approaches. This new material combination strategy may play an important role in the development of an attractive new class of solution processable gate dielectrics.

Keywords: Organic Field-Effect Transistors, Operation Voltage, Energy Efficiency, Flexible Electronics, Low-Bandgap Semiconductors, High-k Dielectrics, Device Engineering.



Biography: Arif Kösemen graduated from AbantİzzetBaysal University, Faculty of Arts and Sciences, Department of Physics in 2006. He received his master's degree from Gebze Institute of Technology, Institute of Engineering and Science in 2010 with the thesis of "Fabrication and characterization of dual-type electrochromic devices with single-wall carbon nanotube in gel electrolyte.". In the following period, he completed the doctorate programs of the same departments with his thesis on "Fabrication and Characterization of Semiconductor Metal Oxide Nano Structures and Inverted Type Hybrid Solar Cell Applications." in 2016 and received his doctorate title. He was awarded the title of associate professor in 2020.

He worked as a research assistant at Gebze Technical University Physics Department between 2010-2016. Between 2016-2022, he served as a researcher at department of Detector and Sensor Technologies in MuşAlparslan University. Also He was the head of the department in the optician program in MuşAlparslan University. Since 2022, he has been working at Istanbul University-

Cerrahpaşa, Institute of Nanotechnology and Biotechnology, Department of Nanotechnology. Research interests are based on fabrication and characterization of organic electronic devices (OPVs, OFETs and ECDs) and gas sensors. He has specialized in fabrication and characterization (XRD, XPS, SEM, AFM) of metal oxide nano-particles (thin film, nano rods, nano tubes etc.) by several methods such as electrochemical, sol-gel, sputtering etc. and application of metal oxide nano materials on inverted type organic solar cells. Also He interest in fabrication and characterization of OFET and Photo-OFET devices.

He hasjoined RD51 research group within CERN with his colleagues to develop new aspects for gas electron multiplier (GEM) foil materials since 2021.

ICRTMD-2023/KT/011 Nnano-Magnetic Oxide Particles and Fluids: Small Size – Vast Applications

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Abstract

Magnetic oxides particles at nano-scale have properties that are much different from their bulk counterpart. However, their properties are very stable over long time and environmental conditions. Owing to their large surface to volume ratio these materials offer potential applications. Using these nano-magnetic particles, magnetic fluids were prepared in which the nano-particles remains suspended in Brownian motion due to thermal agitation at room temperature. These fluids are very stable against gravitational and strong magnetic forces over a long period of time. The low frictional properties of ferrofluid bearings around the poles of permanent magnets were studied and it has been found that the ferrofluid bearings provides a low frictional path to the magnet motion with coefficient of friction equal to 0.0008. This makes the motion of the magnet quite easy and thus provides us a way where we can utilize this property in the design and development of high efficiency wind tubing. By reducing the torque, we are increasing the rotational speed and hence generating the more output electric power at same input wind power. Using these properties of nano-magnetic oxide particles and fluids following industrial applications were explored:

- Energy Sector: In Wind Turbines
- Sensors: Temperature/vibration/acceleration, humidity/alcohol, contactless sensing etc.
- Memory storage: Single domain and Multiferroic materials
- Magnetic Cooling: Self cooling, Transformer core
- **MEMS:** Micro-valve, micro-pump
- EMI Shielding: Microwave absorption.

Keywords: Nano, Magnetic fluids, Ferrofluid bearing, Sensors, Self-cooling.



Biography: Dr. Vinod Kumar is working as Associate Professor in Physics at Department of Physics, NetajiSubhas University of Technology, Dwarka, New Delhi. He had been working in the field of nano-materials specially on the synthesis, properties and device applications of nano-magnetic particles and ferro fluids in energy and sensor devices. His work has good industrial applications. Dr. Kumar has more than 90 publications in International Journals of repute. Two patents have been granted to him and two more has been published. Five students have completed their Ph.D. degree in his supervision and four more are going on. He has received research awards from National Physical Laboratory, New Delhi; International Union of Radio Sciences and Indian National Science Academy. He has been actively involved in the research projects granted from various funding agencies like DST, UGC, UGC - DAE etc.
Jaculty / Scientist (Invited) Talks

Impact of various co-solvents on the micellar behavior of ionic surfactants

Ashwani Kumar Sood

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Abstract

Surface-active agents (surfactants) and their micellar characteristics are considerably on trend for their solicitations in industrial, pharmaceutical, drug delivery and much more, that largely rely on the solvent system in which they are utilized. Therefore, various additives as well as co-solvents are incorporated to the surfactant preparations to enhance their surface characteristics. Addition of co-solvents to the surfactant solutions bring out many changes in the micellar behaviour, which mainly occurs due to some modifications in the solvent structure and surfactant aggregates. The development of micelle mostly relies on the hydrophobic nature of surfactants as well as solvent. Due to this, it is very significant to analyze the role played by solvent media in order to figure out the micellization phenomenon.

Herein, the interactions of different types of surfactants in the presence of solvents including deep eutectic solvents and electrolytes have been discussed along with various micellar, thermodynamic and physicochemical parameters using different techniques at varying temperatures.

Keywords: surfactant; Critical micelle concentration; co-solvents; micellar parameters.

Mathematical modeling for the assessment of antifouling property of biogenic synthesized nanocomposite film

Zeenat Arif

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Abstract

Green synthesis of Nanoparticles is gaining interest as they depict environmental friendly properties thus avoiding use of toxic chemicals and impregnation of these inorganic particle as filler has become a versatile approach in improving the antifouling characteristics of material. In this study, nanocomposite film was prepared using filler as Titanium Dioxide (TiO₂) NPs prepared via extract of Cajanus Cajan (Pigeon Pea). Quantitaive and qualitative analysis was carried out to assess the fouling phenomenon of prepared nanocomposite film by corelating the impact of biogenic synthesis of NP addition on the surface charge, that is, contact angle to interfacial interactions that prevail between foulants and TiO₂ immobilized surface and were evaluated mathematically based on the extended Derjaguin–Landau–Verwey–Overbeek (XDLVO) approach. This theory predicts an increase in strength of repulsive interactive energy barrier with an increase in TiO₂ loading. For qualitative analysis, antimicrobial property of particle against Gram-negative E. Coli (Escherichia coli) was conducted and it was concluded that particle possess excellent antimicrobial property.

Keywords: Antimicrobial; Fouling; Nanoparticle; Surface charge; Wastewater.

Tuning Gas Sensing Properties in Chemically Synthesized Zinc Oxide-Doped Cadmium Sulfide Nanocomposites through Annealing Effects

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Abstract

Gas sensing materials play a vital role in various industrial and environmental applications, where the efficient detection of specific gases is of paramount importance. In this research, I've offered an overview and combination of Zinc Oxide (ZnO)-doped Cadmium Sulfide (CdS) nanocomposites tailored for gas sensing applications. The nanocomposites were prepared using a chemical synthesis method and underwent optimization through annealing processes. The study begins with the chemical synthesis of ZnO-doped CdS nanocomposites, carefully controlling the dopant concentration and the nanocomposite morphology. The effect of temperature during annealing and duration on the morphological and structural characteristics of the nanocomposites is investigated. The optimized annealing conditions are determined to enhance the gas sensing properties. The gas sensing characteristics of CdS nanocomposites doped with ZnO are systematically evaluated under various gas atmospheres, including common industrial pollutants. The nanocomposites exhibit promising gas sensing capabilities, demonstrating sensitivity and selectivity towards specific gases. The results indicate that the annealing process significantly influences the gas sensing performance, leading to improved response and recovery times, as well as enhanced selectivity and stability. This research highlights the importance of controlled annealing in tailoring the gas detection properties of ZnO-doped CdS nanocomposites. The results provide valuable insights for the development of advanced gas sensors with enhanced performance and offer potential solutions for real-world gas detection challenges in industrial and environmental settings.

Keywords: Nanocomposite, morphology, precipitation, sensor, TEM.

Investigating optical properties of biomass waste derived carbon quantum dots prepared by hydrothermal method

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Abstract

The 0D Carbon quantum dots (CQDs) or simply carbon dots (CDs) is one of the new class of hybrid carbon nanomaterials family. These quantum dots have diverse applications in the fields of biosensing, chemical sensing, bioimaging, photocatalysis, electrocatalysis, fluorescent probes, drug delivery, therapy, and many more. The CDs are also known as nanolights or fluorescent carbon nanoparticles for their excellent optical properties. The state of Assam is world famous for tea manufacturing industries and the wastes produced in the tea industry can be converted to value-added products. The main objective of this work is to convert biomass waste into a useful product. Here, we have synthesized CDs from tea waste biomass through a hydrothermal route using phosphoric acid as an activating agent collected from a tea garden near our college. The fluorescence properties of these CDs were also thoroughly investigated by excitation at different wavelengths. The characterization of prepared CDs was carried out by using UV-visible spectroscopy, FTIR spectroscopy, XRD, and TEM image analysis. These carbon nanoparticles show green fluorescence properties of these CDs in different optical sensing applications for hazardous pollutants.

Keywords: Carbon dots (CDs), Biomass, Optical property, Hydrothermal method, TEM.

ICRTMD-2023/FIT/SIT/106 Synthesis and Characterization of Copper Ceria Oxide Nanofibers for Catalyst & Wastewater Treatment

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Abstract

In present study composite CuO/CeO₂ nanofibers containing 10, 20, 30, 40, 50 and 60 mol. % Cu as well as pure ceria were successfully prepared using sol-gel and electro-spinning technique from solutions containing polyvinylpyrrolidone (PVP), cerium nitrate hexahydrate and copper acetate monohydrate. The electro-spinning was carried out at 12kV DC by maintaining the tip to collector distance as 10 cm. The green nanofibers thus obtained were calcined at 500oC for three hours. The morphology of the synthesized nanofibers (both green and calcined) was determined by SEM analysis and their elemental composition was verified using XPS, EDX spectroscopy and other characterization for functional groups (FTIR), thermal stability (TGA). The average diameter of the green composite fibers was found to be in the range of 98-130 nm, while that of the calcined ones was in the range of 78-98 nm. The crystal structure of nanofibers was determined by X-ray diffraction (XRD) which showed the peaks of CeO₂ appearing at 20 of 28.83° and those for CuO at 47.45°. The average crystallite size of CeO₂ and CuO/CeO₂, calculated by Debye-Scherer formula, were found to be 14 nm for CeO₂ and 9-12 nm for CuO/CeO₂ composites of different copper loadings. The application of these nanofibers in catalyst and environment.

Keywords: catalyst, Copper/ Ceria, environment, nanofibers, Synthesis.

Synthetic Textile Polymers and Their Modifications

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Abstract

A large variety of synthetic fibres are used in textile production use namely polyester (55%), polyamide or nylons (5%), polyacrylic (2%), polypropylene, polyurethane etc., the percentages are being in respect of total fibre production. The advantage of the synthetic fibres are that they can be widely modified to match the specific requirements of the enduses. Polyester can be made hydrophilic and comfortable by suitable modifications. Normal polyester fibres are difficult to dye. A number of modified polyesters are now available such as Deep dyeable polyester (DD-PET), cationic dyeable polyester (CD-PET), texturising and draw texturing of partially oriented yarn (POY). Carrier-free dyeable polyester (CFDP). Nylon 6 and nylon 6,6 are two commonly used types of polyamide fibres. Nylon is popular for its strength, lustre, elasticity and resistance to damage by oil and chemicals. Aramid or aromatic polyamide fibres namely Nomex and Kevlar possess very high thermal stability and flame resistance. The acrylic fibres include acrylic, modacrylic and other vinyl fibres containing cyanide groups as side chains. The fibres containing more than 85% and less than 85% acrylonitrile are known as acrylic, and modacrylic fibres, respectively. Acrylic fibres have found a wide spectrum of use where soft, wool-like characteristics are desired. Polypropylene is one of the most versatile polymers produced commercially, with applications both as a plastic and fibre. Polyurethane based spandex (e.g. Lycra®), having high elasticity (400% stretchable), the most popular choice for clothing of high flexibility like sports apparel, swimwear, etc. Polymer based textile composites are used for automobiles, construction, aerospace and composites. Biopolymers offers the advantage of being derived from renewable resources such as corn, sugar, starch, and other bio-based materials. These gained interest for biomedical applications.

Keywords: Synthetic textile fibres, polyester, nylons and acrylic fibres, polylkenes and polyurethenes, modified synthetic fibres, biopolymers.

ICRTMD-2023/FIT/SIT/110 DFT Study of Molecular Interaction of Curcumin with Silver Nanocluster

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Abstract

The molecular interaction between curcumin, a naturally occurring polyphenolic compound with numerous health benefits, and silver nanoclusters has been investigated using Density Functional Theory (DFT). Silver nanoclusters are of great interest due to their unique optical, electronic, and catalytic properties. Understanding the interaction between curcumin and silver nanoclusters at the molecular level is crucial for potential applications in drug delivery, bioimaging, and therapeutics. DFT calculations have been used to explain the experimental observation such as UV-visible and IR frequencies. A detailed elucidation on the density of state calculation has been reported explaining that curcumin not only serves as a reducing agent or stabilizing agent for silver nanoclusters but also activates the nanoparticle by reducing the band gap in silver nanoparticles.

Keywords: Silver nanoparticles, curcumin, molecular interaction, DFT calculation

ICRTMD-2023/FIT/SIT/116 A Novel Spectrophotometric Method for Rapid Quantification of Oseltamivir Phosphate Using Dithiocarbamate Complexation

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Abstract

Oseltamivir phosphate (OSP) is crucial for treating swine flu (H1N1 influenza), and ensuring its purity is essential to prevent adulteration-related health risks. In view of emerging scenario of adulterated pharma products around the globe there is dire need of innovative methods for the rapid and precise quantification of oseltamivir phosphate (OSP). The current spectrophotometric method involves the conversion of oseltamivir into dithiocarbamate through a reaction with carbon disulfide, followed by the formation of a distinct yellow complex with copper acetate. Through extensive optimization, the method demonstrates high sensitivity, adhering to Beer's law over a broad concentration range. Notably, the approach ensures instant and stable color development without the need for product extraction. This cost-effective and user-friendly method requires no specialized equipment or high-level expertise, making it ideal for routine quality control applications in both bulk and pharmaceutical dosage forms. Importantly, the method overcomes the limitations of acidimetric techniques, enabling precise determination of amine-based drugs like OSP even in the presence of interfering basic compounds.

Keywords: Oseltamivir phosphate (OSP); Dithiocarbamate; Spectrophotometric method.

X-ray Absorption Spectroscopy (XAS) for the local structure determination of nanodimensional materials

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Abstract

Synchotron-driven X-rays have led to the development of innovative types of X-ray spectroscopy, especially Xray absorption spectroscopy (XAS), which provide information about the energy-dependent absorption spectrum of a particular atom. The absorption spectra depend on the physical and chemical state of the absorbing atom and its local environment which can be probed by XAS, using two techniques, X-ray absorption near-edge spectroscopy (XANES) and extended X-ray absorption fine structure (EXAFS) spectroscopy. XANES discloses the oxidation state and local environment, while XEAFS provides the number, type, and distances of other atoms bound to it. In the present talk, our recent results on the structural and chemical environment of nanodimensional systems in the form of nanomaterials and multilayer/thin films studied by XAS will be discussed. We will present our results on Eu, Ni, Mn, Co, and Li doped in different nanomaterials like ZnO, Gd₂S₃, BAM, ZnFe₂O₄, BaTiO₃, etc. along with structural information on Co/Ti multilayer, MgO/Co/MgO, Fe/Cr/Al, ZnCoO/ZnO heterostructures.

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Keywords: XAFS, XANES, Nanomaterials, Thin films, Multilayer.

Fabrication of metal chalcogemide /p-Si NW heterostructured thin films for advanced applications

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Abstract

Semiconductor heterojunctions fabricated over one-dimensional nanowire templates are predicted to hold high prospects as compared to bulk heterojunction because of smaller carrier collection distance often comparable to the minority carrier diffusion length. One-dimensional (1D) vertically aligned Si NWs have shown promising potential with enhanced performance owing to their large interfacial area and providing vectorial pathways for charge transport. It also provides an excellent template for the fabrication of diverse heterojunctions. Metal chalcogenides are promising candidates for photocatalysis and sensing devices. Metal chalcogenide/p-Si NWs are expected to exhibit enhanced device efficiencies because of efficient charge separation at the interfacial region. We have successfully synthesized CdS/p-Si NW hetero-junctional device for moisture enabled electricity generation. This primitive module can be utilized as a future energy generation device and can be commercialized by constituting individual units connected either through simple series or parallel connection to scale up high electrical power. We are also exploring other combinations like PbS/p-Si NW and ZnO/p-Si NW for sensing and anti-microbial applications respectively.

Biography of presenting author: Sucheta Sen Gupta completed her Ph.D (2013) in chemistry under the supervision of Prof. Somobrata Acharya and Prof D.D. Sarma at Indian Association for Cultivation of Science, Kolkata, India. As a post doctoral fellow, she joined Prof. Yuval Golan group at the Department of Materials Engineering, Ben Gurion University, Israel and continued there for almost three and half years (March,2013-July, 2016). She then joined the Department of Physics, Mumbai University, India as an DST Inspire Faculty Fellow in India from (2017- 2018). After that, she moved to Amity Institute of Advanced Research and Studies (Materials and Devices), Amity University, Noida and since than shae has been working there. Her present research interest includes chemical bath deposition of metal chalcogenide thin films for application in the photovoltaics, photothermal and sensing devices.

ICRTMD-2023/FIT/SIT/120 Resistive Switching in RF-Sputtered HfOx Based Random Access Memories with Low Switching Voltage!!!

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Abstract

Hafnium oxide (HfO₂) is one of the multifunctional binary oxides which has attracted tremendous research interest due to its potential applications in resistive switching based random access memory (RRAM), ferroelectric RAM (FeRAM) and as a high-K dielectric in CMOS devices. In this work, we present a detailed study on resistive switching in different temperatures processed HfO₂ thin films based metal (Au)-insulator (HfO₂)-metal (Pt) (MIM) devices for RRAM application. HfO₂ films were deposited at room temperature on platinized silicon substrates by RF magnetron sputtering. Rapid thermal annealing (RTA) of the sputtered films was carried out at different temperatures $(400^{\circ}C - 700^{\circ}C)$ in nitrogen atmosphere. Phase and crystal structure of the films were studied using X-ray diffraction. Surface morphology and elemental composition of the films were studied using a Field emission gun scanning electron microscope (FEG-SEM) along with electron dispersive xray spectroscopy (EDS). Atomic force microscopy was employed to analyse evolution of morphology and surface roughness, X-ray photoelectron spectroscopy was used to study chemical composition of the films. Resistive switching behaviour was studied using tungsten microprobes connected to a source meter. Bipolar resistive switching with SET and RESET state currents as low as 700 µA and 70 µA respectively with the wide distribution in VRESET as compared to the VSET were observed. These devices exhibit exceptional electrical characteristics, including stable and repeatable resistive switching (RS) and a significantly low switching voltages (about VSET~0.2 V and VRESET~-0.4 V). In addition to stable retention for more than 103 s, HfO_x thin films possess good endurance upto 500 cycles at low read voltage of 0.5 V. The charge transport mechanism was explained by linear fitting of I-V characteristics, which reveals that LRS is dominated by Ohmic conduction for all voltages and HRS by Space Charged Limited Conduction (SCLC) behaviour at higher voltage. Moreover, the devices recorded good OFF/ON resistance ratio ~ 10 makes it promising candidate for RS memory applications. Moreover, with increase in annealing temperature, the leakage current in HfOx films initially decreases and then increases.

Keywords: Resistive switching, Memory, Memristor, Conduction, Annealing.

Photocatalytic application and Cyclic Voltammetry Study of Nickel Pyrophosphate Nano-Particles

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Abstract

Nickel pyrophosphate (Ni₂P₂O₇) is an interesting material with use in energy storage devices and supercapacitors. The surfactant – mediated approach is used to synthesis nickel pyrophosphate nano particles and further analyzed by using Powder XRD and TEM for confirmation of nano-structured nature. Methylthioninium chloride or popularly known Methylene blue (MB) organic dye is chosen for the photo-catalytic study using nickel pyrophosphate nano-particles. Due to large industrial use the MB is found in wastewater and hence the decomposition of MB has become a degradation standard practice. For photo-degradation of MB by nickel pyrophosphate nano-particles is confirmed through several analyses, viz., wastewater analysis, total organic carbon (TOC) analysis, ion chromatography and UV -Vis. The results indicate that MB degrades in lower molecular leuco-dye. This gives an important application of synthesized nickel pyrophosphate nano-particles in an organic pollutant removal. To evaluate the electro-chemical properties of nickel pyrophosphate nanoparticles are found to be potential photo-catalysts for MB dye degradation. The cyclic voltammetry study was carried out to ascertain the application potential for supercapacitors.

Keywords: Nickel pyrophosphate nano-particles, photo-catalytic activity, Wastewater treatment, Dye degradation, EIS spectroscopy.

ICRTMD-2023/FIT/SIT/124 Reduction in Environmental Electromagnetic Pollution using Conjugated Polymers

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Abstract

The era of modern technology demands to increase the utilization of electromagnetic energy for various miniaturized and complex devices in the field of aerospace, military, industries and scientific level. Therefore, the enhancement in electromagnetic energy and utilization of electromagnetic devices increase the electromagnetic pollution across the earth which directly or indirectly affect the human life as well as performance of electronic devices. To overcome this problem caused due to electromagnetic devices/radiations, the efficient shielding materials are required to protect the working performance of electronic devices. To eliminate the electromagnetic pollution from the environment, the optimized use of magnetic and dielectric losses as they are capable to shield the electromagnetic devices from the electromagnetic pollution by the reflection and absorption mechanisms. Normally, the absorption dominant shielding materials are suitable than reflection for the protection of electronic devices as reflection further may lead to interference effect to nearby devices. Moreover, the combination of conducting and magnetic materials is much suitable for the good absorbed shielding material. A study from the last two decades indicates the utilization of nanocomposites of conjugated polymers with highly conducting or magnetic materials contributed significantly to shield the electromagnetic radiation because of these materials exhibit tremendous properties such as easy to synthesized, cost effective, light weight, non-corrosion, etc. Also, from two dimensional materials, MXene, graphene, CNTs contribute significantly in the electromagnetic shielding performance. The shielding properties are generally investigated in terms of total attenuation in energy/power of incident electromagnetic waves i.e., called total shielding effectiveness (SET). If the value of SET is very small i.e., below 10 dB that means materials have no shielding but if the values lie between 10 to 30 dB that means minimum effective shielding. However, if this value exceeds than 30 dB that signifies that best efficient material for industrial application.

Keywords: Electromagnetic Shielding; Conjugated Polymers; MXene; Nanostructures; Attenuation.

ICRTMD-2023/FIT/SIT/127 Catalyzing Sustainability: Transesterification with Heterogeneous Catalysts for efficient Biodiesel Production

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Abstract

Biodiesel is an alternative, renewable and clean-burning fuel and obtained from biological sources such as vegetable oils or animal fat. Chemically, biodiesel is fatty acid methyl ester (FAME) and produced through a chemical process called transesterification in which triglycerides (fats and oils) mix with an alcohol (commonly methanol or ethanol) in the presence of a catalyst to produce biodiesel and glycerol. The use of catalysts is crucial in accelerating this reaction and making it industrially viable. Transesterification can be facilitated by the use of both homogeneous and heterogeneous catalysts. Heterogeneous catalysts are advantageous for biodiesel synthesis transesterification due to their ease of separation, recyclability, reduced environmental impact, operational flexibility, and stability. These factors make it possible to produce biodiesel more efficiently and sustainably. The synthesis of biodiesel can be achieved with heterogeneous catalysts such as metal oxides, sulfated metal oxides, zeolites, and immobilized lipase. The selection of catalyst is influenced by factors like the specific reaction conditions, feedstock characteristics, and the desired properties of the biodiesel product.

Keywords: Renewable fuel; Heterogeneous catalysts; Transesterification; Biodiesel.

ICRTMD-2023/FIT/SIT/128 Polyscharide polymer-linked Barium sulphate nano material for selective tumor cell diagnosis and treatment

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Abstract

The use of stable carrageenan nanoparticles linked to barium sulphate for specific organ functions as well as imaging contrast to aid in diagnosis. This study investigated the ways in which barium sulphate interacts with the polysaccharide component of carrageenan, as well as the ways in which K-linked iota carrageenan is linked to Ba^{2+} ions. Ion replacement and carrageenan rheology were used to connect the Ba^{2+} ion to activities that were already fighting tumours. Since the Ba^{2+} ion can both diagnose and fight tumours, it was necessary to connect it to these activities. Carrageenan possesses properties that help with tracing and imaging target selectivity. These properties include biological selectivity, targeted selectivity, and cancer selectivity. The investigation revealed that there is a robust interaction between the cation Ba^{2+} and the anion sulphate, which prevents the substance from dissociating and renders it hydrophobic. This indicates that it will no longer form gels and will instead be able to form stable nanoparticles without the requirement of cross-linking agents. Nanoparticles, thanks to their enhanced fluorescence activity, are better suited than conventional particles for imaging and targeting cells within organ systems. They could be utilised for precision medicine, fluorescent light, and X-ray/CT imaging due to their high pKa value and the fact that they release Ba2+, which prevents cells from osmosis and kills cancer cells.

Keywords: Carrageenan; Natural Polymer; Polysaccharide; Barium linked carrageenan Nano particle; Contrast media; Diagnosis agent; selective anti-tumor diagnosis and treatment.

Exploring a Spectrum of Size and Shape Effects: Melting Point and Lattice Parameter Dependencies in Gold and Copper Nanoparticles

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Abstract

In our preceding exposition, we posited an empirical nexus between the melting points of nanostructured materials and their bulk counterparts. In this study, we introduce a method to determine the fraction of surface atoms relative to the total number of atoms within a nanoparticle. This method utilizes a distribution approach for surface and interior atoms within the unit cell of a nanomaterial crystal, and the derived fraction is linked to the size and shape of the nanomaterial. Additionally, we develop a proposition that correlates the relaxation factor with the presence of dangling bonds in surface atoms, based on the ratio of surface atoms to the total atoms. Subsequently, we estimate the melting points for coinage metals like gold, and copper across various nanoparticle sizes and shapes. Our revelations exhibit a commendable concordance with experimentally ascertained values for these particles. Apart from melting point, the lattice parameter of a nanocluster also depends on surface energy and size along with the shape of the particle. In the present undertaking, the size and shape dependencies of the lattice parameter of nanoparticles are scrutinized within the framework of our extended model, building upon our antecedent research work. The modulation of lattice parameters concerning various sizes and shapes of gold and copper nanoparticles is estimated, and a comparative analysis with extant data is undertaken. Our results harmonize effectively with experimental findings, underscoring the robustness of our proposed model.

Keywords: Melting point, Lattice parameter, Nanoparticle, Size, Shape.

ICRTMD-2023/FIT/SIT/130 Defect Rich Carbon Nanostructures Based Hybrids: Possible Cold Cathodes in Electron Microscope

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Abstract

Carbon has always found its importance in various fields of applications since the advent of material science and this trend found a new boom with the emergence of concepts of nanoscience and technology in the end of the last decade. The material, carbon is really a wonder since whenever the researchers thought that the properties of material is wellmanifested it showed a completely new phase and thus different sets of properties. Carbon can exist in different hybridization states of completely contradictory properties. In nano-regime carbon can exists in all possible four-dimensional forms like carbon dot (0 D), carbon fibre (1 D), carbon sheet (2 D) or other different structures (3 D) and thus the charge confinement effect is best visible in such system. Carbon nanostructure founds its application in different fields including hydrophobic coating, sensor, single electron transistor, gas storage device, supercapacitor, hydrogen generator and many other. One of such important application is emission of electron under the influence of electric field which is called cold field emission (FE). Cold FE can result significant energy savings by lowering the threshold voltage needed for electron emission by the mechanism of field enhancement. The reason behind this, stands on the fact that unlike the conventional thermionic emission of electron the field emission is a purely quantum mechanical phenomena and here the supplied energy can be much lesser compared to the work function of the material as here instead of jumping over the barrier the electron basically comes into the vacuum by a process of tunnelling. This talk will discuss the cold emission characteristics of different carbon nanostructures and related hybrids and more specifically the talk will deal the effects of defects in the synthesis of carbon-based hybrids and hence the cold emission properties of carbon nanostructures.

Keywords: CNT, Graphene, Cold Emission, Nanostructures, Field enhancement, Work function.

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ICRTMD-2023/FIT/SIT/131 Potential of Pharmaceutical Nanotechnology in the management of Neuro AIDS

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Abstract

The inability of ARV drugs to go across the blood-brain barrier (BBB) after systemic administration makes the brain one of the dominant HIV reservoirs. The practice and investigation of nanomedicine possesses potentials for therapeutics against neuroAIDS. This lecture will highlight the advancements in pharmaceutical nanotechnology to design and develop nanoARTs for efficient delivery across BBB so as to recognize and eradicate HIV brain reservoirs.

ICRTMD-2023/FIT/SIT/133 Guiding Selection of Correct Ingredients to Realize Host Sensitized Dopant Emission

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Abstract

Doped semiconductor nanoparticles (NPs) offer a promising ground to generate novel luminophores that potentially can benefit from individual properties of the host and dopants. Trivalent lanthanide cations (Ln^{3+}) doping are particularly attractive in this regard due to the unique emission properties of these cations. An appropriate semiconductor NP can act as a sensitizer and protector matrix for Ln^{3+} emission, necessities associated with an extremely inefficient direct excitation and environmental quenching effects. Systematic investigations on the II - VI sulfide and selenide NPs identify terbium doped zinc sulfide NPs being an efficient system. These observations are rationalized based on a charge trapping mediated dopant emission sensitization process, in which an optimum positioning of dopant ground and luminescent energy levels with respect to the valence and conduction bands of the NP is of extreme importance. The lanthanide emission lifetimes in inorganic NPs are found to be biexponential, where the shorter and longer lifetime components are correlated with lesser and more protected surface and core sites of the NPs, respectively. A systematic comparison and analysis of these lifetimes in the NPs with that of in molecular complexes and freely floating ions identify that the lengthening of emission lifetime in inorganic NPs arises irrespective of operation of an optical antenna effect and that this lengthening associates with access to all inorganic core in the NPs. The charge trapping mediated dopant emission sensitization mechanism is verified by undertaking experiments with band gap matched NPs and in various oxides. The understanding from these f-block doped semiconductor NPs is generalized to d-block elements doped zinc sulfide NPs. Collectively, these analyses identify a recipe to predict the correct host (semiconductor NPs) - guest (dopant) pair in order to generate optimum host sensitized dopant emission in a predictive way, rather than attempting this by a trial-and-error approach.

Keywords: Doping, Semiconductor nanoparticles, Photoluminescence, Sensitized emission, Charge trapping.

Valorization of Dried Flowers of Medicinal Plant into Natural Dye

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Abstract

Natural dyes are currently used as eco-friendly and biodegradable products in the textile industry. In this work, dried flowers of Azadirachta indica RUBL21378 and Acacia Catechu RUBL20387 were collected and extracts were prepared in different organic solvents like methanol, ethanol, and acetone. These extracts were enriched with saponins, quinone, flavonoids, and alkaloids after phytochemical screening. They showed antimicrobial activity with good zone of inhibition against growth of Escherichia coli, Staphylococcus aureus, Pseudomonas aeruginosa and Bacillus cereus. Natural dyes were synthesized for cotton fabrics using different metallic mordant (copper sulfate/ferrous sulfate), bio-mordant (green tea). Cotton fabrics dyed with bio-mordant based natural dye showed better stability in detergent solution and high temperature. The color fastness was observed after treating them with sunlight at different interval of time period for 24, 48, and 72 hours. The cotton fabrics showed stability in detergent solution (2%) for 30 minutes at 50°C. These fabrics showed equal color intensity after dyeing with green tea as mordant. Scanning electron microscope and FTIR peak analysis had confirmed the entrapment of dye across cotton fabrics. These natural dyes could be efficiently employed in textile industry to color fabrics at large scale.

Keywords: Acacia, Azadirachta, Flower, Antimicrobial property, Natural dye.

Sol-gel derived Fe-doped ZnO NPs: Structural, Morphological and Magnetic Properties

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Abstract

Zinc oxide nanoparticles are very catalytically active and have a considerable surface area compared to their size. Depending on how they are created, zinc oxide nanoparticles can have a variety of specific physical and chemical characteristics. The following processes can be used to make ZnO nanoparticles: laser ablation, hydrothermal methods, electrochemical depositions, sol-gel method, chemical vapour deposition, thermal decomposition, combustion methods, ultrasound, microwave-assisted combustion method, two-step mechanochemical-thermal synthesis, anodization, co-precipitation, electrophoretic deposition, and precipitation processes using solution concentration, pH, and washing medium. At ambient temperature, the energy gap of the wide-bandgap n-type semiconductor ZnO is 3.37 eV, and the large exciton binding energy of about 60 meV, which makes it a promising material for short-wavelength optoelectronic applications. Transition metal doped ZnO behaves as a diluted magnetic semiconductor (DMS) which has been under intense research due to its potential applications in spin-based multifunctional electronic devices. In this work, $Zn_{1-x}Fe_xO$ (x = 0.00, 0.10, 0.20, and 0.30) NPs were synthesized using the sol-gel method. X-ray diffraction confirmed that $Zn_{1-x}Fe_xO$ NPs have a wurtzite hexagonal structure. The average crystallite size was found in the range of 16.01 to 19.73 nm. Williamson-Hall's method detected the tensile microstrain. Fe-doped ZnO nanoparticles have cauliflower-like surface morphology confirmed by FESEM. Magnetic measurement (VSM) indicated diamagnetic to ferromagnetic transition and enhancement in saturation magnetization (Ms from 0.3234 to 3.6927 emu g⁻¹) with an increase in Fe content.

Keywords: ZnO NPs; X-ray diffraction; Diluted magnetic semiconductor (DMS); FESEM; VSM.

ICRTMD-2023/FIT/SIT/143 Conductometric method for the determination of corrosion of Aluminium metal in hydrochloric acid medium

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Abstract

Conductivity measurement has widespread use in industrial applications, which involve the detection of ionic contaminants in water and concentration measurements. The electrochemical corrosion monitoring techniques such as polarization techniques, potentiometric methods and galvanic sensors are complicated and require particular expertise in using nitrogen gas for isolation the solutions from oxygen. Unlike the other electrochemical techniques, the electrical conductivity method is available simple and not affected by oxygen pressure and its results are easy to interpret. In addition, among the techniques recently developed, electrochemical noise tests have proven to be beneficial as a method of determining the corrosion rate of certain passive materials, although scientists are striving to interpret conflicting results. The basis for the electrical conductivity approach is the fact that materials with higher electrical conductivities facilitate the flow of electric current more readily than those with lower electrical conductivities. An essential characteristic of materials is electrical conductivity, which is influenced by the type of material, its structure, the temperature, and the presence of impurities or imperfections. In the present study corrosion of aluminium is measured in acid medium with and with out inhibitor.OCP, weightloss measurements were also employed to study the inhibitor mechanism. All these study showed that presence of corrosion inhibitor in the medium lowers the corrosion rate of the metal.inhibition efficiency of the inhibitor increses with concentration.

Keywords: Conductometric method; Aluminium corrosion; Open circuit measurement; Weightloss measurement; Drug as inhibitor.

ICRTMD-2023/FIT/SIT/144 Solution-processed UV-visible-Near Infrared (NIR) broadband Photodetector based on ZnO/CH₃NH₃PbI₃ heterojunction

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Abstract

This paper presents a succinct report on ZnO Nanoparticles (NPs)/CH₃NH₃ PbI₃/PTB₇/MoO₃/Ag-based UVvisible-Near Infrared (NIR) broadband photodetector fabricated on the fluorine-doped tin oxide (FTO) coated glass substrate. ZnO NPs layer acts as the electron transport layer (ETL), CH₃NH₃PbI₃ acts as the active layer, PTB7 acts as the hole transport layer (HTL) and MoO₃ is used to optimize the recombination current in the proposed photodetector structure. The spin coating method has been used for depositing the layers of ZnO NPs, CH₃NH₃PbI₃, and PTB₇ in the proposed structure while the MoO₃ layer has been grown by the thermal evaporation method. The optical measurements over the 350-850 nm wavelength range give the maximum photoresponsivity, detectivity, and external quantum efficiency (EQE) of ~0.36 A/W, ~7.8x10 12 Jones, and ~83.67 % under -2 V, respectively. The proposed photodetector gives a rise time and fall time of 81 ms and 75 ms, respectively.

Keywords: CH₃NH₃PbI₃, EQE, perovskite, photodetector, PTB7, UV-visible-NIR, ZnO NPs.

Development of metal-oxide nanostructured interphase in basalt fiber reinforced polymer composites for structural applications

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Abstract

Surface treatment of woven basalt fibers were performed to growth zinc-oxide nanostructures seed-mediated solvo-thermal deposition technique. Different functional groups were developed on fiber surface to increase the potential bonding site for polymer matrix while fabricating composites. The optimal value of process parameters such as seeding cycles, growth temperature, growth duration and molar concentration were evaluated for uniform growth of nanostructures on fabric surface. The basalt fabric samples were uniformly coated with zincoxide featuring a wurtzite structure and hexagonal nanorods morphology. The growth of well-aligned zinc-oxide nanorods on basalt fabrics were achieved at 6 seeding cycle, 6 hours of growth duration and 100 °C growth temperature in a 30 mM concentration of growth solution. The crystallinity, morphology, and compositional attributed of the pristine basalt fabrics and ZnO-coated basalt fabrics were evaluated using X-ray diffraction. field emission scanning electron microscopy, and energy-dispersive X-ray spectroscopy. The final composite samples were fabricated by reinforcing ZnO-modified basalt fabrics with epoxy resin matrix using vacuum bagging method. The samples were further tested under drop down impact tester and micro-UTM for studying their mechanical properties and it was observed that the samples exhibit appreciable increase in the impact energy absorbance capacity, elastic modulus, tensile strength, and in-plane shear strength due to enhanced interfacial properties. Based on these results, the developed hybrid composites exhibit promising properties for applications in industries such as aircraft and automobile manufacturing. They offer high impact strength, high modulus, lightweight characteristics, and low void content, making them desirable materials for these industries.

Keywords: Surface treatment; Basalt fabrics; Zinc-oxide; Nanostructures; Solvo-thermal process; Impact strength; Nanocomposites.

ICRTMD-2023/FIT/SIT/147 Nanomaterials-based Electrochemical Sensors for p-Phenylenediamine (An organic dye)

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Abstract

p-phenylene diamine, a constituent of hair dye and also used in coloring textiles and polymeric fibre industries. Its long exposure to humans can cause several problems related to skin or respiratory organs. It was also found that it causes too many cancer-causing effects. The water sources near the manufacturing units get polluted with p-PDA-containing wastewater causing destruction towards aquatic fauna. Hence, the monitoring of p-PDA concentration in products as well as wastewater coming from manufacturing units should be done. The electrochemical method is a very easy and cost-effective technique to develop a sensor towards the detection of p-PDA in samples. A few literature reports are available in this regard.

In the last two years, our group have tried to develop some such nanomaterial-modified electrochemical sensors for the detection of p-PDA in different samples. We obtained satisfactory results in real samples in terms of selectivity, sensitivity, calibration linear range limit of detection etc.

Keywords: Nanomaterial, p-Phenylenediammine, Sensor, Electrochemical.

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ICRTMD-2023/FIT/SIT/150 Displacement Sensor by Conventional Optical Fiber with Different Reflectometer for dissimilar Media

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Abstract

Light-intensity-modulated displacement sensors are extensively used in numerous applications. Such type of sensors operate by utilizing a pair of adjacent optical fiber's and a reflector. Such displacement sensors have the benefits of higher sensitivity and operating range, because they can efficiently collect more light after a reflectance has occurred. The light-sensing behaviour of these two cases is mathematically modelled, giving sensing characteristics such as linearity and sensitivity. Experimental results are presented for verification and validation of the models. By the use of different reflectometer intensity modulation has been done with respect to different propagating media. Apart from this, changing medium also influences the intensity profile of light that guided to the receiving fiber. Out of all the reflectors, convex mirror yields the maximum output with respect to different varying medium. In all four medium enhanced with different refractive indices, concave mirror emerges to be the best candidate for displacement sensor. Additionally the results are found to be matching with simulated one and exhibit good repeatability over a wide range. Key words: Light-intensity-modulated displacement sensors, single optical fiber, optical fiber sensor, Intensity Modulation.

Polumer Based Detectors Throw Light on Astroparticle Physics and Medical Physics

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Abstract

DEASA (Dayalbagh Educational Air Shower Array) consisting of eight plastic scintillators each with an area of 1 square meter to measure the secondary cosmic rays. The cosmic ray showers have been simulated in CORSIKA [1] for the different primary particles in the energy range of 10^{14} - 10^{15} eV. The longitudinal and lateral profile has been studied for Agra. The real-life applications of cosmic ray particles in space have been studied to protect the astronaut from the solar energetic particles and galactic cosmic rays [2]. A plastic scintillation detector is simulated in Geant4 to study applications in hadron and carbon ion therapy [3]. The proton and carbon beam are simulated through the tumor region to study the stopping power and depth dose distribution for different organs. The energy range for each study is optimized and Bragg curve is then interpreted with Bragg peak position and range. Another application of secondary cosmic muons is to be able to scan the radioactive container has also been studied with the help of Monte-Carlo simulations (Geant4) [4] which is called muon tomography. In this study, a dry cask container has been simulated which contains the UO₂ rods and the muon scattering has been observed [5]. This is the basic concept behind muometric wireless navigation system (MuWNS).

Keywords: Polymer scintillation detector; air shower; CORSIKA; cancer studies.

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ICRTMD-2023/FIT/SIT/156 Synthesis of Proton Exchange Membranes for Microbial Fuel Cell

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Abstract

A Microbial fuel cell (MFC) is bio-electrochemical type of fuel cell which converts the chemical energy present in organic compounds to electrical energy. These systems are the emerging field and have some advantages over electrochemical cell because they do not emit polluting gases like CO, SO₂ etc. They can be used for biohydrogen production, wastewater treatment, environmental sensors and bioremediation. The system consists of two-chamber partitioned by a separator. The separator is one of the most important factors in an MFC, and it has a significant effect on its performance. A proton exchange membrane (PEM) is the most frequently used separator in MFCs due to its moderately high conductivity to protons and low internal resistance compared to other separators. Now-a-days, various research groups are focusing on development of PEM based fuel cell commercially which will be able to reduce the use of present oil and gas based fuel and decrease the pollution. PEM based on polymer gel electrolytes have received attention because of its high conductivity and its ability to conduct electricity in solid as well as aqueous medium. The present work deals with the synthesis of PEM by using different concentrations of SiO₂ and and phosphotungstic acid (PWA) with an aim to get the high conducting membrane. Their application in microbial fuel cell was also studied.

Keywords: Proton exchange membrane, separator, water uptake, Phosphotungstic acid, Microbial Fuel Cell.

Green Synthesis and Photocatalytic Activity of Chitosan coated Iron Oxide Nanoparticles

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Abstract

Iron oxide nanoparticles (Fe_2O_3 NPs) were synthesized through a biogenic approach using Pelargonium graveolens leaf extract with the addition of ferric chloride due to their non-toxicity and environmental friendly behavior. Spectral analysis of UV-VIS and FTIR showed the presence of Fe₂O₃ NPs. Chitosan is used to coat the synthesized iron nanoparticles. Congo Red (CR) dye solution was prepared in the concentration of 100 ml (0.02%) for decolonization studies. The synthesized iron oxide nanoparticles showed excellent photocatalytic activity under UV light at a wavelength of 595 nm. Chitosan iron oxide nanoparticles and free Chitosan were used to decolourize the CR dye. Using Chitosan, the maximum decolourization was observed of 0.02% concentrations of CR dye solutions with 0.03% of chitosan. It accounts for 82.25% in CR dye in 0.03% of aqueous solutions of chitosan after decolourization. Using iron oxide nanoparticle chitosan, the maximum decolourization was observed of 0.02% concentrations of CR dye solutions with 0.03% of chitosan iron nanoparticle composite. It accounts for 85.5% of CR dye in 0.03% of aqueous solutions of iron nanoparticle chitosan composite after decolourization. Antibacterial activity of the iron nanoparticles was assessed towards pathogenic bacteria such as Bacillus subtilis, Pseudomonas aeruginosa, Enterobacter aerogenes and Klebsiella pneumonia. The synthesized Fe₂O₃ NPs showed more bactericidal activity against Klebsiella pneumonia with 11mm of the zone of inhibition using 100ul of iron oxide nanoparticles. Because of promising activity, iron oxide nanoparticles Chitosan composite could be used for the degradation of dye and Pelargonium graveolens leaf extract can be applied as an eco-benign and cost-effective approach for the synthesis of Fe_2O_3 NPs.

Keywords: Green Synthesis; Iron oxide nanoparticles; Chitosan; Congo Red Dye; Photocatalytic.

ICRTMD-2023/FIT/SIT/167 Biosynthesis of Silver Nanoparticles Using Psidium cattleianum Leaf extract and their Antimicrobial activity

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Abstract

The present study was to analyze the phytoconstituents, bioactive compounds present in Psidium cattleianum leaves, to synthesize Silver nanoparticles from the leaves extract and to evaluate their anti-microbial property. The plant P. cattleianum commonly known as strawberry guava. The phytochemical analysis of leaf extracts of various solvents showed the presence of alkaloids, phenols, flavonoids, saponins, terpenoids, cardiac glycosides and sterols. Aqueous extract of strawberry guava leaves showed the highest phenol, flavonoid content with the value of 60.5 mg GAE/g and 57.0 mg QE/g whereas lowest was observed in ethanol of as 14.2mg GAE/g and 32.4 mg QE/g respectively. Silver nanoparticles were synthesized and visible colour change was observed. Uv-Vis spectrum of the synthesized AgNPs showed band at 436 nm and the crystalline nature of the AgNPs was confirmed by XRD analysis. The FTIR spectrum revealed the presence of functional groups such as alcohols, phenols, carboxylic acids, alkene, alkanes, amines and amides. These may belong to the bioactive compounds in the plant extract that aided as stabilizing, reducing and capping agent. The TEM micrograph showed that particles were majorly spherical in shape with very less agglomeration and the average size of the synthesized nanoparticle was 20 nm. Ag NPs exhibited potential antimicrobial activity against C. albicans (26 nm) when compared to crude extract. GC-MS analysis of the extracts was done to identify the important bioactive compounds present in them which were responsible for their biological activity.

Keywords: Psidium cattleianum; Anti-microbial; AgNPs; Bioactive compounds; Flavonoids.

Effect of doping on CuCrO₂ prepared by solid state reaction method

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Abstract

Owing to significant P type conductivity and transparancy, Delafossite materials have gained the increased scientific interest in recent years. These materials exhibit promising potential in various applications such as photovoltaics, sensors, and transparent electronics. This paper presents a detailed account of the synthesis of polycrystalline $CuCrO_2$ delafossite in pure and doped forms via the solid-state reaction method. The effect of doping with 5% Magnisium and Strontium has been examined. The structural properties of the sample were analyzed using X-ray diffraction which confirms rhombohedral crystal structure with R-3m space group. The variation in peak intensities and positions has been analyzed and attributed to variation of ionic radii. Grain size and lattice parameters have been caluclated. The Effect of doping on optical properties has been examined using UV-visible spectroscopy. Reduction in the band gap with doping has been attributed to the creation of extra energy levels.

Keywords: Delafossite, Transparent Electronics, Solid State Reaction Method, Doping.

ICRTMD-2023/FIT/SIT/178 Development of Triboelectric Nanogenerators for self-powered sensing application

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Abstract

Recently, energy harvesting strategies through human daily activities are being investigated worldwide. Conversion of the bio-mechanical energy into electrical energy is an unique approach to power up small sensors or gadgets for daily life use. In this context, Triboelectric nanogenerators (TENG) have evolved as potential devices as they are compatible with a wide range of active materials. Again, the dependence of output on external factors like temperature, humidity and the chemical environment brings the scope of deployment of the TENG devices as self-powered sensors. In the present talk, the sensing characteristics of various TENG devices will be discussed [1-3]. The varying output of TENG through biomechanical movements can serve as motion sensor. Particularly, the sweat and motion sensing application of TENG composed of chemically grown zinc oxide (ZnO) nanostructures on flexible platform will be introduced. Further the application of ZnO based nanocomposite for temperature sensing will be addressed. Finally the introduction of machine learning techniques for recognition of the signals generated through the biomechanical movement of TENG will also be highlighted.

Keywords: Energy harvesting; nanogenerator; nanocomposite; sensing.

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3-D conductive metal organic frameworks (MOFs): Next generation conductive materials

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Abstract

Four isostructural formate based conductive MOFs namely, $[H_2N(CH_3)_2][M(HCO_2)_3]$ (M = Mn, Co, Ni, Zn), were synthesized with simple and cost effective methods. The in situ generated formate ion was attributed to decomposition of DMF under high pressure and temperature. As-synthesized MOFs exhibit impressive room temperature electrical conductivity which is attributed to the charge flow along the pores of the MOFs and electron flow through the metal-ligand bond owing to metal d-orbital and ligand p-orbital overlap. Upon removal of guest from the pores the electrical conductivity of all the frameworks were improved except for MOF with cobalt metal centre. The formation of highly mobile hydronium ion upon removal of guest may be one of the reasons of improvement in the conductivity of aforementioned de-guested MOFs. The theoretical evaluation of band of the MOFs reveals that through bond conductivity is significantly determined by the number of high spin electron in the metal d-orbitals.

Keywords: Conductive MOF; Formate anion; In-situ formation; Through Bond; Transistion Metal.

Experimental Investigation of Optical and Nanocooling Features of Silver Nanoparticles-Graphene Hybrid Material

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Abstract

The stronghold state of graphene has enabled scientists and technologists to find applications of this vital material in almost every domain of walks of life, owing to the multifaceted function it performs [1]. The generation of heat due to two rubbing surfaces is a common process occurring in most the machine elements and some time the rise in temperature is detrimental to the component [2]. The development of highly thermally conducting fluid is the need of the future developments in efficient cooling systems. The optical properties of graphene had also been explored ever since graphene was discovered, which include absorption and transmittance, application in light emitting devices [3], and recently it has attracted tremendous interest for its application in surface enhanced Raman spectroscopy [4, 5]. In the present contribution, water and ethylene glycol based highly efficient thermally conducting nanofluid was prepared and its properties and performance were evaluated. Silver nanoparticles-graphene based hybrid material was developed as efficient heat transport nanomaterial additive. To get a stable suspension, the ultrafine silver nanoparticles of size < 20 nm have been synthesized. The synthesized hybrid nanomaterial has been characterized by various characterization techniques such as TEM, XRD, TGA, Raman spectroscopy, FT-IR spectroscopy, UV-Vis spectroscopy etc. The thermal conductivity analysis of nanocoolant developed shows very promising results and exhibits the thermal conductivity enhancement by 20%, with respect to base fluid (equivalent to commercially available coolant composition), which shows its potential to be used as an efficient coolant. The extensive Raman spectroscopic analysis of hybrid nanomaterial was also investigated and shows it's potential for application in Surface Enhanced Raman Spectroscopy (SERS), which is well illustrated, and this promises another application of this hybrid nanomaterial for sensors.

Keywords: Silver Nanoparticles-Graphene hybrid, D/G ratio, Nanocoolants, Thermal Conductivity.

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High-Performance SERS Substrates for Biomolecular Detections

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Abstract

Sensing systems with creative capabilities are increasingly crucial, especially with the growing significance of plasmon-induced Surface-enhanced Raman scattering (SERS) in trace detections. The utilization of metallic nanostructuring offers an innovative method for transforming incident free-space light into a localized electromagnetic field within confined spatial dimensions. Customizing the confined electromagnetic field of the substrate to particular regions at designated excitation wavelengths serves as a potent strategy for improving the SERS enhancement factor, thereby advancing the efficacy of single molecular assays. In this work, diverse metallic nanostructures designed for optimal operation within the near-infrared (IR) spectrum are investigated as promising platforms for surface-enhanced Raman scattering and refractive index sensing applications. The plasmonic enhancements in both near and far fields of the nanoarrays are carefully adjusted to optimize the overall performance. The near-field characteristics demonstrate the generation of a robust electric field at the tips and gaps of the structure, leading to improved Raman scattering. This phenomenon results in SERS enhancement factors ranging from 10^9 to 10^{11} . Conversely, the far-field characteristics indicate significant modifications in extinction spectra, coupled with changes in the permittivity of the ambient environment, suggesting potential applications in various sensing scenarios. The augmentation of Raman signal intensity and refractive index sensitivity is achieved through the optimization of geometrical parameters, gap dimensions, and symmetry. The study explores the performance of arrays comprising crisscross nano dimers and hexagonal nanodisks, with asymmetric tuning of sizes and varying spatial orientations, to enhance detection limits. Results underscore the SERS activity and refractive index sensitivity of different Gold/Silver nanostructures, exhibiting enhanced performance at shorter wavelengths and demonstrating compatibility as reliable substrates for practical applications.

Keywords: Plasmonic nanostructures; Surface-enhanced Raman scattering (SERS); Enhancement factor; Refractive index sensing.
ICRTMD-2023/FIT/SIT/184 Structural, Optical and Magnetic Properties of Transition metals doped Metal Oxide Nanoparticles

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Abstract

Semiconducting metal oxide nanomaterials (SMO) are prominent materials for scientific and technological advancement in nanoelectronics, optoelectronics, photovoltaics, magneto-optics, magnetoelectronics, and photonic devices. These materials act differently than bulk semiconductors due to their distinct chemical, physical, electrical, and magnetic properties [1]. Nanoparticles of tin oxide (SnO2) doped with transition metals were synthesized through the chemical precipitation method. The powder X-ray diffraction patterns of pure and doped samples showed tetragonal rutile structure and crystallographic space group (p42/mnm) (136), consistent with the standard JCPDS File Nos. 41-1445 and 96-152-6638. The band gap energy value for 1 M of pure and doped transition metals exhibits a blue shift, whereas for 2 M and 3 M of pure and transition metals, doped SnO₂ nanoparticles shifted to a higher wavelength (red-shift) compared to bulk SnO₂ (3.65 eV). PL emission peaks at 655 nm were observed, revealing an increased intensity for the peak attributed to O-vacancies and a small red-shift and in its position due to dopant atoms possibly incorporating in the host SnO2 lattice. In comparison, Sn_{0.97}Mn_{0.03}O₂ and Sn_{0.97}Fe_{0.03}O₂ samples have a high coercivity and retentivity was recorded to 7372 Oe and 773 emus, 7191 Oe and 666 emus respectively.

Keywords: Co-precipitation, PXRD, Optical, Photoluminescence, Ferromagnetism.

Effect of POSS Hybrid Nanomaterials and MXenes on Solid Polymer Electrolytes for Rechargeable Lithium Batteries

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Abstract

For lithium batteries, solid polymer electrolytes (SPEs) have been seen as a successful way to remove the majority of possible safety concerns associated with traditional liquid electrolytes. Utilizing improved comprehensive performance SPE systems, such as plastic crystal, poly(ethylene oxide), polycarbonates, polyhedral oligomeric silsesquioxane (POSS), polyphosphazene, and MXene-based SPEs, has been the focus of extensive research efforts. POSS/MXene-based SPEs are among the best options available for SPEs because of their easy chemical alterations, superior thermal and chemical stabilities, and low glass transition temperatures (Tg). However, despite significant advancements in this area, POSS/MXene based electrolytes continue to face several difficulties and struggle to fulfill the demands of real-world uses. Furthermore, to the best of our knowledge, there aren't many distinct and indepth studies on the development of POSS/MXene-based SPEs, particularly in the more recent advancements for lithium batteries after 2010. In this study, we provide a thorough overview of the development of POSS polymer, POSS ionic liquids, POSS lithium salt, and MXene-based electrolytes, as well as their possible uses in solid-state lithium-ion batteries from the standpoints of ionic conductivity, electrochemical properties, and modification techniques.

Keywords: POSS Hybrid Nanomaterials; MXene; Solid Polymer Electrolytes; Ionic Conductivity; Rechargeable Batteries.

ICRTMD-2023/FIT/SIT/187 Temperature dependent electric and magnetic properties of Pr doped BTO-NFO coreshell multiferroic nanocomposite

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Abstract

In the present study, we have investigated the structure, morphology, temperature dependent dielectric, ferroelectric and magnetic properties, and ME coupling of MnNFO-PrBaTiO₃ core-shell nanocomposite synthesized by the combination of co-precipitation and sol-gel method. The XRD spectra revealed that the ferroelectric BT phase is compatible with the magnetic MnNFO phase. Scanning Electron microscopy (SEM) and Energy-Dispersive X-ray spectroscopy confirmed the formation of core-shell like structure in the composite. The magnetic and ferroelectric phase preserves their basic individual properties in the core-shell form. The temperature dependence of dielectric permittivity showed a sharp phase transition from cubic to tetragonal structure of the core-shell composite at 292 K. Frequency dependent dielectric study shows an enhanced value of permittivity (14000) along with low dielectric losses. It was found that the prepared composite exhibited moderate values of saturation magnetization (23.84 emu/g) at 293K and polarization (5.146 μ C/cm²) along with low remnant polarization at room temperature. Moreover, we also observed enhanced energy storage efficiency (67%) which are explained due to strong interfacial coupling and reduced leakage current, making this composite promising for multifunctional device applications.

Keywords: Core shell, sol-gel, multiferroic, energy storage device, hysteresis loop.

ICRTMD-2023/FIT/SIT/189 Enhanced Photocatalytic Activity of Gd³⁺ Doped ZnO Nanoparticles for Malachite Green Dye Degradation

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Abstract

Gd-doped ZnO (Gd_xZn_{1-x}O, where x = 0.00, 0.03, 0.06, 0.09 and x = 0.12) with rich oxygen vacancy defects was synthesized by co-precipitation method. The formation of hexagonal wurtzite structure of ZnO and Gd doped ZnO was confirmed by X-ray Diffraction (XRD). Energy Dispersive X-ray (EDX) analysis shows the presence of zinc, gadolinium, and oxygen in stoichiometric ratios. SEM images showed a mixed morphology of spindle and spherical particles upon doping. Optical band gap energy calculated from the UV–visible absorbance spectra of the samples was found to be ~3.32 eV. Photoluminescence (PL) and Raman spectroscopy reveals the presence of various surface defects in the Gd doped samples with $Gd_{0.06}Zn_{0.94}O$ possessing maximum oxygen vacancy/zinc interstitials related defects. $Gd_{0.06}Zn_{0.94}O$ also exhibits the best photocatalytic activity towards the degradation of malachite green (MG) dye among the doped samples. Under the optimized conditions of $Gd_{0.06}Zn_{0.94}O$ load = 0.35 g/L; dye concentration = 10 ppm and dye solution's pH = 10, degradation percentage increases from 96% in 3 hrs. 30 min without optimization to 99% within 10 min of irradiation. Scavenging activity study revealed that electrons play major role in the photocatalyst was found to decline gradually in the consecutive runs which needs to be overcome by a suitable solution.

Keywords: Semiconductor materials, Oxidation, Materials degradation, Nanomaterials.

Silicon nitride (Si₃N₄) anti-reflection coating thin film on silicon using chemical vapor deposition (CVD) techniques

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Abstract

Thin films of silicon nitride have been useful in various semiconductor technologies for very large scale integration, transistor, and anti-reflection coating (ARC) in solar cell applications. Because of their unique physical, chemical and electrical properties which is highly remarkable and significant. In this report silicon nitride (Si_3N_4) thin films are successfully deposited on silicon (p-type) substrate by using chemical vapor deposition (CVD) techniques at 800°C. The prepared Si3N4 thin film, reflectance, structural, functional and morphological properties were investigated using UV- Visible spectrophotometer (UV-Vis), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and atomic force microscopy (AFM). UV-Visible spectroscopy revealed the lowest reflection up to 15%, which is better performance as an ARC. The enhanced anti-reflection coating properties due to the combination of Si and N source chemistries (flow rate) and vapor phase growth process parameters. The AFM (3D) topology image of scanning surfaces is 1x1µm2 and obtained results in the height (thickness) of 25 nm, 4.2 nm, and 24.2 nm with the corresponding surface area ratio of 2.8, 2.2 and 2.3%.

Keywords: Thin film; CVD; Si3N4; AFM; Anti-reflection coating; XRD.

Sol-Gel Synthesis of La-SnO₂ NPs for Efficient Removal of dyes in Wastewater Treatment

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Abstract

The simultaneous elimination of antibiotics and heavy metal contaminants from wastewater without causing secondary contamination and with easy recovery presents a significant challenge. In order to tackle this issue, we employed a straightforward sol-gel method to prepare SnO₂-based photocatalysts, with the goal of achieving high-value reuse and promoting environmental protection. The formation of nanoparticles was confirmed through analysis using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and High-resolution transmission electron microscopy (HRTEM). Raman and XPS spectroscopy were utilized to explore electronic, optical properties, and lattice defects. The incorporation of dopant La into the La-SnO₂ nanoparticles demonstrated remarkable catalytic performance, breaking down 94% of a 10 ppm RB dye solution within 60 minutes of UV light exposure. Even after four cycles, the catalytic degradation activity remained high at 87%, indicating excellent structural stability. This enhancement can be attributed to an increased adsorption capacity and efficient separation of electron-hole pairs under light illumination. The results underscore the potential of these composites as effective materials for breaking down harmful organic pollutants in wastewater treatment offering promising possibilities for environmental remediation and advanced technology.

Keywords: Photocatalysis, SnO₂, Rare-earth doping, Magnetization, RB dye.

ICRTMD-2023/FIT/SIT/202 Methodology used for crystallization kinetics, optical properties and electrical behavior of heavy metal doped glasses

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Abstract

The crystallization kinetics, optical absorption spectra and electrical behavior of lithium cadmium silicate glasses with varying amount of bismuth content were investigated using non-isothermal crystallization approach and UV-VIS-NIR spectroscopy. These glasses were synthesized by normal melt quenching technique. The crystallization kinetics for the glasses was studied by using the Kissinger and modified Ozawa equations. Appearance of a sharp cut-off, and a wide and reasonable transmission in VIS-NIR regime makes them useful for optical applications such as IR transmission window. The cut-off wavelength, optical band gap and Urbach's energy have been analyzed and discussed in terms of change in the glass structure. By analyzing the impedance spectra, the ac and dc conductivities, activation energy for dc conduction (Edc) and for relaxation frequency (EM") were calculated. The results obtained from dc conductivity confirmed the network forming role of Cd2+ ion in the glass. The scaling of the conductivity spectra has been used to interpret the temperature dependence of the relaxation dynamics. The observed conductivity spectra follows power law with exponent 's' which decreases with temperatures and satisfied the correlated barrier hopping (CBH) model. The perfect overlying of normalized plots of electrical modulus on a single 'master curve' depicts temperature as well as composition independent dynamical process at several frequencies.

Keyword: Bismuth silicate glass; DSC; Impedance spectroscopy; Optical band gap.

Potential of solid supported copper catalyst in sustainable organic synthesis

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Abstract

Heterogeneous metal catalysis has gained importance in the last decade as it offers advantages like reusability of the catalyst, ease of separation, minimum metal contamination in product and economical as well as environmental sustainability. Heterogeneous copper catalyst has been developed with an aim to study the efficiency of supported copper on synthetic organic reactions leading to useful molecules which are important components in pharmaceutical chemistry. The methodologies involving heterogeneous copper catalysis leads to sustainable alternative pathways to the synthesis of drug molecules as well as other biologically relevant moieties. This review will include the synthesis and application of copper catalysts supported on several different solid supports like hydroxyapatite, titanium dioxide, silica etc. The review will highlight the use of these solid supported copper catalysts in useful organic reactions. The aim of this article is to develop a platform which will guide future organic chemists towards developing newer methods of heterogeneous catalysis for sustainable organic synthesis.

Keywords: Copper; Heterogeneous; Sustainable; Organic synthesis; Reusability.

ICRTMD-2023/FIT/SIT/205 Synthesis of cellulose-based materials for sensing and environmental remediation

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Abstract

Cellulose-based materials have gained significant attention in the field of sensing and adsorption due to their unique properties, including biocompatibility, renewability, and environmental friendliness. Cellulose nanocrystals can be used in various types of sensors such as gas sensors, humidity sensor due to their high surface area and the ability to functionalize their surfaces for specific detection. Also, Cellulose nanocrystals possess a large surface area and can be used as adsorbents for water purification. They can effectively remove pollutants, such as heavy metals and dyes, from water. Various modifications on the surface of cellulose and nanocellulose can be performed to imrove its sensing and adorption efficiency. Herein, we report various functionalizations and nanocomposites preparation of cellulose nanofibers. The synthesized composties of cellulose materials have been used for developing sensors for environment contaminants and also as adsorbent to remove environment contaminants through adsorption.

Keywords: Cellulose, cellusoe nanofibers, sensing, adsorption, environmental remediation.

Polymer Membranes for Separation Application

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Abstract

Membrane technology is the leading technology for all kinds of separation techniques due to its intrinsic characteristics such as operational simplicity, environmental impact, high selectivity, and permeability for the transport of specific components. Membranes have been employed for the separation of gases and liquid-liquid mixtures through microfiltration, reverse osmosis, ultrafiltration, pervaporation, gas separation, dialysis, and nanofiltration. Membranes could be fabricated from inorganic and organic materials. Zeolites, ceramics, and metal materials are used to design membranes for separation technology owing to their good separation performance and high mechanical, thermal, and chemical stability. However, the difficulty in manufacturing a defect-free membrane and the cost of production limits its application in separation technology. Ease of availability, processability, low operation cost, and tunable properties could make polymer membranes a promising material in the separation arena. Polymer membranes are extensively used to separate a particular component from a mixture of gases or vapours. The main challenge in membrane separation technology is to overcome the trade-off effect between permeability and selectivity. To tackle this problem, one promising strategy is the introduction of fillers to get mixed matrix membranes (MMMs). Various polymers such as polyimides, poly vinyl alcohol, polysulfone, polyamides, polyaniline, cellulose acetate polyarylates, polycarbonates and poly (phenylene oxide) are employed as a selective membrane for the transport of liquids and gases. The presentation is on the applications of polymer membranes and MMMs in the separation of gases and water purification.

Keywords: Membranes; gas separation; water purification; mixed matrix membranes.

ICRTMD-2023/FIT/SIT/208 Kelvin Probe Force Microscopy (KPFM) study on Antibacterial Behaviour of Graphene Oxide nanohybrid

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Abstract

Bacteria can easily attach to biological and non-biological surfaces and they fetch the nourishment from such surfaces and does their metabolic activities. The attachment and the growth of the bacterial colony compromise the proper functioning of the surfaces. Many a time the failure of equipments, like the eye lenses, prosthetic attachments, artificial bones, heart valves, dentures etc.are noticed due to the bacterial infections. Apart from the bodily risk, bacteria also possess threats to the beverages industries, food industries, water purification processes, sanitation etc. Surfaces with different materials such as Cu, Zn, TiO2 etc. are tried but failed to be potent materials towards antibacterial activities and mere results in their accumulation as waste. In this context graphene based materials have been used extensively as a potential alternative for the antibacterial therapy. In this research, we have shown the death mechanism of the bacterial cell over the synthesised composite of zincphthalocyanine-graphene oxide (ZnPc-GO) thin films with the help of Kelvin Probe Force Microscopy (KPFM) which is a very powerful analysis to show the temporal changes of the bacterial cytoplasm during dying. KPFM helped in quantifying the mechanism of cell death with the help of measuring (mapping) the transfer of charges in the vicinity due to the generated ROS-exhibited-stress at the bacterial and composite interface. A time dependant study shows a clear picture of leakage of cytoplasm which contains the lipopolysaccharide that deals with bacterial surface potential. Since the charge transfer from bacterial cell happens to be an irreversible process, the cell dies and the charge spread in terms of cytoplasm leakage. We are sure that the study will uncover the mechanism of the death bacterial cells by quantification of the change of surface charges.

Keywords: ZnPc-GO nanohybrid, KPFM, Anti-bacterial activity, ROS-exhibited stress, surface potential.

Structural and Electrical changes investigations in aged copper sulphate doped poly (otoluidine)

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Abstract

The aging effect on the conductivity and structural properties of poly (o-toluidine) prepared via chemical oxidative polymerization with potassium dichromate as an oxidizing agent and resulted doped with copper sulphate in different concentrations is the subject of present investigation. Electrical conductivity measurements obtained using two probe method on doped poly (o-toluidine) composites shows different behavior compared with two years old measurements with same dopant concentrations in pellet form as well as in powder form. However the analysis of samples by XRD, exhibits and confirm the change in structural form of composites from semi crystalline to amorphous one as with aging irrespective of doping concentrations.

Keywords: Poly (o-toluidine), DC Conductivity, XRD pattern, Aging effect.

Augmented healing of full thickness chronic excision wound by antimicrobial loaded chitosan encapsulated graphene nanocomposite

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Abstract

Nanoparticles have become pivotal in wound treatment due to their ability to facilitate sustained and effective topical delivery of antimicrobial drugs. Incorporating active excipients like chitosan or graphene oxide during formulation enhances the potential for chronic wound healing. In this study, we designed, fabricated, and assessed antimicrobial-loaded chitosan-encapsulated graphene nanoparticles (AN-CH-G-NPOs) to augment wound healing. The nanoparticles underwent thorough characterization through particle size, Zeta potential, FT-IR, SEM, TEM, and AFM analyses. The optimized formulation was integrated into Carbopol gel and subjected to evaluations encompassing drug content, pH, in vitro release, texture analysis, and viscosity. The antibacterial activity against Staphylococcus aureus was determined through minimum inhibitory concentration. In vitro antimicrobial activity was assessed using a microdilution assay. Furthermore, in vivo evaluations on Sprague Dawley rats demonstrated the wound healing efficacy of the fabricated nanocomposite. Histopathological analyses revealed significant improvements in wound contraction, cell adhesion, epithelial migration, and hydroxyproline content, indicating enhanced collagen synthesis. This study underscores the potential of topically administered fabricated nanocomposites as a promising strategy for treating chronic wounds.

Keywords: Nanoparticles, Graphene oxide, chitosan, wound healing.

ICRTMD-2023/FIT/SIT/216 Antimicrobial, anti-fungal and anticancer activity of N-(5-(N-((Z)-2-((Z)-(((5-acetamido-1,3,4-thiadiazol-2-yl)sulfonyl)imino)methyl)-6-methoxyphenoxy)dioctylstannyl)oxy)-3methoxybenzylidene)sulfamoyl)-1,3,4-thiadiazol-2-yl)acetamide

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Abstract

This research work was aimed at developing a potent drug which could act as an antibacterial agent, antifungal and anticancer agent. A novel complex has been synthesized successfully by using two methods: The conventional method of refluxing and the microwave method, where the reaction mixture was exposed to microwave radiations in a domestic microwave oven. The microwave method is observed to be more efficient and rapid than the conventional method because the amount of yield obtained is greater in the case of the former and also the reaction time is quite less. The product formed was collected by filtration and dried in a vacuum. The synthesized complex was characterized using spectral analysis (UV-Vis absorption, FTIR technology, 1H NMR, 13C NMR, and 119Sn NMR studies). The data obtained from 119Sn NMR spectra confirmed the proposed geometries in complexes where the ligand were found to coordinate to tin metal through (O) and (O,N) donor sites. The novel complex has shown good antibacterial, antifungal and anticancer in in-silico docking studies.

Keywords: A potent drug, Novel complex, Spectral analysis, Antibacterial, in-silico docking studies.

Architecture of inorganic-organic hybrid perovskites for enhanced stable photovoltaic performance

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Abstract

The current study focuses on the advancement of thin film-based perovskite solar cells by taking into account the most important factors such as degradation, instability, and toxicity, all of which are undesirable for perovskite photovoltaic technology. In this research work, we have successfully fabricated lead (Pb)-replaced and Pb-free perovskite solar cells at ambient conditions and developed a new fabrication route for highlyefficient and air-stable perovskite solar cells. The carcinogenic Pb has been replaced at ambient conditions under excess chlorine (Cl)-rich system to minimized the degradation tendency of Pb-free perovskite solar cells. The Pb-replaced perovskite solar cells have been further annealed at different annealing conditions to investigated the effect of annealing temperatures on the photovoltaic performances which led to the formation of nanostructured-perovskite solar cells. The investigation showed that the formation of nanostructures is a function of annealing temperatures. The thermal engineering study under excess Cl-rich system have shown positive influences on the stability, surface morphology, structural crystallinity, optical properties, and photovoltaic performance of Pb-replaced perovskite solar cells. The thermal engineering study has influenced to develop a new fabrication route called dual-step thermal engineering technique for developing a highly-efficient and stable methylammonium lead iodide (CH₃NH₃PbI₃)-based perovskite solar cells at ambient conditions. The detail investigation has shown that newly developed dual-step thermal engineering technique is potential over the conventional one-step spin coating method as the new method exhibited remarkable improvement in efficiency and stability of perovskite solar cells. To understand the fundamentals of perovskite's crystalline structure, all of the perovskite thin films and photovoltaic devices were thoroughly investigated using various characterization techniques, as well as Rietveld refinement simulation studies using FullProf. software.

Keywords: Perovskite; solar cells; refinement; thermal engineering.

ICRTMD-2023/FIT/SIT/221 Cadence Virtuoso Based Circuit Simulation of Universal Logic Gates: A Broad Tutorial

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Abstract

Gate-level designs and circuit simulations are fundamental processes for building complex digital circuits. This paper focuses on the design and circuit simulation of two universal digital logic gates viz. NAND and NOR gates using Cadence Virtuoso software. The study leverages the versatile ADE L environment for transient analysis performed on each logic gate to simulate the output response to an input pulse signal. The results of the simulations were plotted as transient graphs to visualize the gate operation properly. The simulated results showed that both NAND and NOR gates were properly operated, which was further validated via their Truth tables. The NAND gate produced only a low output signal, when both of the input signals were high. The NOR gate produced an output signal that was high only, when all of the input signals were low. Through rigorous simulation and meticulous analysis, this research uncovers the dynamic behavior of these logic gates, shedding light on their functionality and performance characteristics.

Keywords: Cadence Virtuoso, ADE L, digital VLSI circuit simulation, transient analysis, NAND gate, NOR gate.

ICRTMD-2023/FIT/SIT/225 Structural, Dielectric and magnetic studies on Al³⁺ substituted ZnAl_xFe_{2-x}O₄ ferrites

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Abstract

ZnAl_xFe_{2-x}O₄ (0.1< x < 0.5) nanoparticle ferrites has been prepared by chemical co-precipitation method to study the effect of Al³⁺ substitution on structural, dielectric and magnetic properties of ZnFe₂O₄ nanoparticles. X-ray diffraction (XRD) and transmission electron microscopy (TEM) images confirmed the nano size formation of particles. The lattice parameter (a), bulk density (ρ m) and X-ray density (ρ x) were found to decrease with increasing inclusion of Al³⁺ ions. AC conductivity (σ ac) measurements as a function of temperature show that the samples behave like semiconductors. Decrease in the hopping conduction between Fe²⁺ \leftrightarrow Fe³⁺ ions at octahedral site is observed with increasing inclusion of Al³⁺ substituted ZnFe₂O₄ ferrites. The magnetization studies revealed that magnetic moment (η _B) showed decreasing trend with increase in substitution of Al³⁺, its value decreases from 0.56 (for x = 0.1) to 0.34 (for x = 0.5). The Ms values decrease from 13.29 emu/gm for x = 0.1 to 8.42 emu/gm for x = 0.5. DM (magnetic particle size) was found to be less than the particle size calculated from TEM micrographs due to presence of magnetically dead layer on the surface of particle. Squareness (S) values infer that particles interact by magnetostatic interactions. The M-H loop of all the samples is narrow with low value of coercivity and retentivity; indicates the superparamagnetic nature of prepared nanoparticles.

Keywords: Structural; dielectric; nanosized; super-paramagnetic.

ICRTMD-2023/FIT/SIT/226 Utilization of agro-wastes as solid substrate for biodegradable PHB production using microbes for sustainable environment

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Abstract

Plastic pollution is causing severe environmental problems for humans, animals, and the whole planet. The pursuit of renewable, resourced, biodegradable materials began in the 1970s, and carbon-neutral, totally sustainable products have driven recent advancements. With ample carbon and limited nitrogen, microorganisms like Alcaligenes, Pseudomonas and Staphylococcus, manufacture polyhydroxybutyrates (PHBs) as energy reserves. These biodegradable biopolymers can replace carbon-based polymers. However, high production costs impede commercialization. This study's primary screening with Sudan black B and Nile Red identified 18 bacterial PHB producers. These isolates were also confirmed by crotonic acid measurement as secondary screening. Sugarcane bagasse has the most cell biomass (33.72 mg/L) and PHB production (23.39 mg/L), followed by potato peel when was screened using solid state fermentation. Placket-Burman design revealed that Urea, KH₂PO₄, and sugarcane bagasse was obtained as significant factors affected KLA09 strain for PHB output, which was further optimized using response surface methods. In FTIR analysis of PHB, O-H (hydroxyl group) at wave number 3925.43 with 55.7% transmittance shows significant bond intensity. C-H bonds are present at wavenumber 2927.28 with a transmittance of 80.5%, followed by C=O, C=C, and C-O bonds at wavenumbers 1659.38, 1546.64, and 1043.40 with 39.2%, 50.9%, and 43.4% transmittance, respectively. This bacterial PHB is showing comparative physico-chemical similarity with the synthetic polymer that makes it a suitable candidate that can cope up with the solid waste management for the sustainable environment.

Keywords: PHB; Biodegradable polymer; Solid waste management; Sudan black B assay; Sustainable environment.

Role of Nd³⁺ substitution on structural behaviour of Bi_{1-x}Nd_xMnO₃

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Abstract

In this study, we have synthesized a series of Bi_{1-x} Nd_xMnO₃ samples using the solid-state reaction method, where the parameter x ranges from 0 to 0.20. Our aim was to investigate the structural and morphological properties of these samples in relation to the varying neodymium doping concentrations. Employing various characterization techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), and Fourier-transform infrared spectroscopy (FTIR), we gained insights into the structural and chemical properties of the prepared samples. X ray diffraction analyses revealed that all samples exhibit an orthorhombic crystal structure with the pbam symmetry. Interestingly, as the neodymium doping level increases, there is a discernible reduction in the overall crystal symmetry, indicative of the influence of higher neodymium concentrations on the crystal lattice arrangement. Furthermore, an intriguing correlation emerged between the neodymium doping and the grain size of the samples, with higher doping leading to a decrease in grain size. This suggests a potential role of neodymium in influencing the microstructural development of the Bi_{1-x} Nd_xMnO₃ samples. Our Fourier-transform infrared spectroscopy results provided further insights into the chemical bonds present within the samples. The FTIR spectra prominently displayed characteristic peaks corresponding to Mn-O and Bi-O bonds. These observations are in consonance with the anticipated perovskite structure of the samples, underlining the robustness of our synthesis approach. In summation, our investigation into the Bi_{1-x} Nd_xMnO₃ samples using X-ray diffraction, scanning electron microscopy, and Fourier-transform infrared spectroscopy has furnished valuable insights. The systematic exploration of varying neodymium doping levels has offered a deeper understanding of the structural evolution, crystal symmetry, and grain size dynamics in these compounds. This study contributes to the body of knowledge surrounding complex oxide materials and lays the foundation for potential applications in advanced electronic and functional device development.

Revolutionizing illumination efficiency in horticulture through rare-earth and transition metal-doped Phosphors

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Abstract

In the realm of contemporary horticulture and plant growth control, the efficient utilization of light plays a pivotal role. This presentation focuses on the synthesis and characterization of phosphor materials doped with rare-earth (RE) / transition metal (TM) ions, with the objective of enhancing their light-emitting properties. The research encompasses the creation and thorough analysis of both singly doped and co-doped phosphor samples, employing a range of characterization techniques.

Our investigation reveals that these doped phosphor materials exhibit robust photoluminescence, which is a critical factor for their potential applications in horticulture lighting. Importantly, in the case of the co-doped samples, it is observed that the emissions of RE and TM ions occur independently, without any mutual quenching or energy transfer mechanisms. This independence is significant as it allows for precise control of the emitted light, a valuable feature for tailored lighting solutions in horticulture.

Overall, the results of our study underscore the considerable potential of the doped phosphor materials for various applications. One of the most promising applications is in solid-state lighting, which can be tailored to provide the specific light spectra required for optimized plant growth. The ability to control and fine-tune the emitted light makes these materials a valuable asset in the pursuit of efficient and sustainable horticulture practices.

Keywords: Phosphors; Horticulture; Light Emitting Diodes; Photoluminescence; Doping; Plant Growth Control.

References:

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Exploration of cost effective earth-abundant metals for enhanced elcrtrocatalytic oxygen evolution reaction

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Abstract

Developing earth-abundant metal based electrocatalyst in place of expensive precious metal catalyst is the always challenge for chemist. Hence herein, we have tried to design the novel molecules and materials using inexpensive earth-abundant metal precursors. In this view, we synthesized and structurally characterized a novel cobalt (II) acetate complex $[(3,5-Lutidine)_2Co(OAc)_2(H_2O)_2]$ as a promising electrocatalyst for oxygen evolution reaction (OER). It was implied that the lutidine will provide coordination flexibility and electron rich environment around the metal center to facilitate the catalytic reaction. Therefore, the as synthesized cobalt complex shows even better OER activity than the state-of-the-art IrO₂ catalyst in terms of turnover frequency (TOF: 0.05) and onset potential (1.50 V vs RHE) under identical conditions. On the other hand we synthesis of a Ni(II) complex [(L)2Ni(NCS)2] as a single source precursor to obtain nickel sulfide nanoparticles (NiS NPs). To improve the electrocatalytic performance and durability, the functionalized multi-walled carbon nanotubes (f-MWCNTs) were used as a support material for Ni-complex. The hybrid between Ni complex and CNTs post-annealing at 350°C resulted in NiS-CNT nanocomposite. The comparison of OER performance in terms of their η 10 values was found to follow the order: Ni-complex<NiS<IrO2<Ni-complex-CNT hybrid<NiS-CNT. This study provides a competent strategy to design OER electrocatalyst using cost effective earthabundant metals.

Keywords: Earth-abundant metals, Co-complex, Ni-complex, MWCNT, OER.

Exploring the applicability of phosphors in various fields

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Abstract

In recent eras, the use of phosphor-converted LEDs has increased daily due to their eco-friendly characteristics. Different rare earth-doped inorganic phosphors drew considerable attention owing to their availability, simple synthesis process, and cost-effectiveness. In the last few decades, the applicability of phosphors has been limited to the fabrication of LEDs and display devices. In recent days, the application of rare earth-doped phosphor material has been studied in various fields such as smart agriculture, recognition of fingerprints and lip print, and anti-counterfeiting as well as in optical thermometry. This talk aims to focus on the study of selection of suitable materials, their synthesis process, and understanding the recent advancement of luminescent materials in above mentioned fields. The next part of the talk deals with the various characterization techniques based on the application, recent work, and their future perspectives.

Keywords: LEDs, fingerprint, anti-counterfeiting, smart agriculture.

ICRTMD-2023/FIT/SIT/235 Photocatalytic degradation of Phenol wastewater by co-doped TiO2 activated carbon nanocomposite

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Abstract

Co-doped titanium dioxide supported on activated carbon (Co-TiO₂@PAC) nanocomposite was synthesized using the hydrothermal synthesis method. The physicochemical characterization of the nanocomposite was done by different analytical methods like SEMEDX, XRD, FT-IR, photoluminescence (PL), pHzpc, and UV-Visible diffuse reflectance spectroscopy (DRS). The visible light active nanocomposite was used for the photocatalytic degradation of phenol from an aqueous solution. The results indicated that the doping of Co ions decreases the bandgap energy, reduces thus improves the visible light photocatalytic activity. The nanocomposite is highly stable and can be used several times without any significant loss of inactivity. GC-MS analysis confirmed the generation of different degraded products like hydroquinone, maleic acid, phenoxide ion, oxalic acid, and formic acid etc.

Keywords: CDT/PAC nanocomposite; Photocatalytic degradation; Phenol; Regeneration.

ICRTMD-2023/FIT/SIT/236 Estimation of Glass Forming Ability and Mechanical Properties of AlZr3 alloy using Molecular Dynamics Simulations

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Abstract

Bulk Metallic Glasses (BMG) also known as amorphous metals are the metallic materials, which have glass like structure, are non-crystalline metal alloys having disordered atomic scale structures. Due to their enhanced structural and metallic properties, the BMGs are one of the prominent fields of research in today's era of scientific developments. One of the key scientific terms used to characterize the BMGs is glass-forming ability (GFA), which is defined as how simple or difficult it is for a BMG to create glass. A number of factors including structural characteristics, temperature, phase diagrams, the formation enthalpy of the amorphous phase of alloys are used to determine the GFA of BMGs. In the present work, molecular dynamics (MD) simulations have been carried out in conjunction with second nearest neighbor modified embedded atomic method (2nn-MEAM) interatomic potential parameters to estimate the GFA of AlZr₃ alloy. AlZr₃ metallic glass specimen is prepared from the molten state by fast quenching process with a cooling rate of the order 10^{12} K/s. The radial distribution function (RDF) curves are obtained at different temperatures during the cooling process and subsequently reduced glass transition temperature of the metallic glass is estimated in order to calculate the GFA. The calculated value of GFA (0.532) and the splitting of second peak into two sub-peaks in the RDF curves mark the formation of good bulk metallic glass (BMG). Further to study the mechanical properties of the BMG, it is subjected to uniaxial tensile stress with strain rates varying from 0.0005 ps-1 to 0.01 ps⁻¹. The decrease in Young's modulus is observed with increase in strain rate. Whereas, the yield strength and yield strain are found to be not perturbed by the change in strain rate. To validate the potential used, the Young's modulus of pure aluminium and zirconium crystals are also calculated with the same potential and a good match between the calculated values with the experimental value is noticed.

Keywords: AlZr₃; BMG; GFA; MD simulations; 2nn-MEAM potential; Young's Modulus.

ICRTMD-2023/FIT/SIT/237 Numerical Analysis of Convection of Nanofluids on Heat Transfer – An Overview

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Abstract

Convective heat transfer inside enclosures utilizing nanofluids and hybrid nanofluids has been numerically investigated by using finite volume method. The simulations focus particularly on the MHD effects, central heater orientation and length, heated wall section length, Rayleigh number, Reynolds number, Richardson number, nanoparticle volume fraction on the average Nusselt number along the cool, vertical side-walls of the enclosure. Regardless of the heater orientation, the heat transfer performance reduces as the magnetic field strength increases.For an increasing different nanoparticle volume fraction, the average Nusselt number increases with an pertinent parameters concerned. Notably, the use of an external magnetic field to control the convection effect has many advantages over traditional active cooling methods, including high reliability, good energy efficiency, a low maintenance cost, and a noise-free nature.

Keywords: Convection; Nanofluids; MHD effect; Heat transfer; average Nusselt number.

ICRTMD-2023/FIT/SIT/240 Comparative Study of Electrical Parameters of Cadmium Telluride and Zinc Telluride Nanoparticles by van der Pauw Hall Measurements

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Abstract

This article elaborates the comparative study of electrical parameters of Cadmium Telluride (CdTe) and Zinc Telluride (ZnTe) nanoparticles. The very easy and less expensive van der Pauw Hall measurement technique is applied to study the electrical properties of CdTe and ZnTe nanoparticles. CdTe nanoaprticles are prepared by Single Injection Hydrothermal method whereas ZnTe nanoparticles are synthesized by Solgel method. The EDAX spectra is taken to confirm the presence of cadmium, tellurium and sulphur (due to the capping agent Thioglycolic acid) in the CdTe nanoaprticles and also to confirm the presence of zinc and tellurium in ZnTe nanoaprticles. The electrical parameters like carrier concentration, mobility, conductivity and type of conductivity are calculated from the van der Pauw Hall measurements. The results show that the the ZnTe nanoaprticles possess good conductivity than the CdTe nanoparticles. However the CdTe nanoaprticles are have high mobility than the ZnTe nanoaprticles. CdTe nanoaprticles are found to possess p-type conductivity whereas the ZnTe nanoaprticles are of n-type conductivity. These interesting electrical properties of CdTe and ZnTe nanoaprticles make them suitable for certain device applications like diode, photovoltaic cells etc.

Keywords: CdTe, ZnTe Nanoparticles, van der Pauw, Hall measurements, electrical properties.

A simple scalable transformation of waste laser toner powder into the magnetic pigment for the development of magnetic leather finishing: An innovative waste utilization strategy

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India

Abstract

Managing e-waste is one of the biggest obstacles to developing a green society. Approximately 6000 tonnes of waste toner powder are produced annually due to the widespread use of laser printers. 35.0% iron oxides, 3.0% SiO2, 55.0% polystyrene, and 7.0% polyacrylate are the main compositions of waste toner. Because of the presence of iron material, it is magnetic. Its chemical and engineering endurance limits its recycling options (20-30%). Due to the lack of reutilization methods, this waste material is frequently disposed of in landfills. Recently, it has been categorised as a potential class-2B carcinogen by the WHO. Finding a new avenue of recycling this waste by turning it into a useful resource is a fantastic way to help the environment. Here, we suggest a simple, scalable thermal conversion of waste toner powder into the magnetic carbon material and subsequently use it as a magnetic black pigment for the development of a magnetic leather finish. The waste toner was ball milled and sieved (> 106 microns) after being meticulously calcined at 600°C under vacuum. Materials were characterised using various analytical tools both before and after calcination. FTIR and XPS demonstrate that calcination enhanced the surface polarity of the magnetic carbon/Fe₃O₄ material by increasing the surface hydroxyl group. Fe₃O₄ was found by XRD in both native and calcined waste toner. FE-SEM revealed that the toner particle's form changes to a spherical, even one following calcination. Fe₃O₄ nanoparticles were recognised by TEM analysis in both the original and modified waste toner. According to a VSM study, calcinations doubles the magnetic nature of the material. Significant magnetic properties are imparted to leather that has been finished with native and treated waste toner using a blend of synthetic and protein binders. Coated leather also demonstrated good abrasion resistance, rub-fastness, and flexing endurance in both dry and wet conditions.

Keywords: Tonner waste, e-waste recycling, magnetic carbon, magnetic leather, green industrialization.

Lamb wave based acoustic devices for wireless sensing applications

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Abstract

The quest for innovation by researchers and engineers has resulted in the creation of diverse sensor types, with acoustic wave-based sensors emerging prominently. These sensors offer numerous advantages, including a stable fundamental frequency, high sensitivity, operation at room temperature, compact dimensions, portability, and prolonged shelf life, along with the potential for wireless integration. Despite the complicated fabrication processes associated with these sensors, their remarkable potential in applications demanding high sensitivity, stability, and reproducibility in remote and challenging environments has been the focal point of this study. Acoustic waves are categorized into Bulk Acoustic Wave (BAW) and Surface Acoustic Wave (SAW), with Lamb wave-based devices within the SAW category demonstrating exceptional mass sensitivity. This is attributed to the entirety of the device being constructed on a membrane, rendering them favorable for sensing applications. Hence, the present study predominantly investigates Lamb wave-based sensors, characterized by sagittal wave propagation and unique features such as antisymmetric and symmetric modes. The exploration extends beyond the fundamental mode to higher modes of the Lamb wave device, leveraging their higher velocity of wave propagation and increased sensitivity to analytes. Theoretical analyses employ finite element analysis, complemented by modeling and simulation techniques using COMSOL Multiphysics software. Optimization discussions revolve around multiple layers of the Lamb wave device to attain a high acoustic velocity and a favorable electromechanical coupling coefficient. In the experimental phase, a piezoelectric ZnO thin film is applied over a SiO₂/Si membrane, and performance studies involve a comparison between experimental and theoretical outcomes. The fabricated Lamb wave devices are further investigated in biosensing, physical sensing, and chemical sensing applications. In biosensing, the Lamb wave devices exhibit notable sensitivity and low detection limits, such as a sensitivity of 310 Hz(ngµl⁻¹)⁻¹ and a detection limit of 82 $pg\mu l^{-1}$ for the fundamental symmetric mode. Similarly, the fundamental antisymmetric mode shows a sensitivity of 202 Hz(ngµ¹)⁻¹ and a limit of detection of 84 pgµ¹. Additionally, the highest mode (A2) of the Lamb wave resonator demonstrates significant sensitivity to UV radiation, with a frequency shift of 535 kHz(mW/cm²)⁻¹ and a high sensitivity of 2.78×10^3 ppm(mW/cm²)⁻¹. The Lamb wave devices, when integrated with metal oxide sensing layers like SnO₂ and ZnO, are further utilized for detecting chemical warfare agents, such as Dimethyl methylphophonate (DMMP) and Dibutyle Sulphide (DBS). Remarkably, the SnO₂ based Lamb wave device shows maximum sensitivity of 4.25 kHz/ppm for DMMP sensing, while the ZnO sensing layer-based sensor exhibits a maximum sensitivity of 2.98 kHz/ppm for DBS sensing.

ICRTMD-2023/FIT/SIT/246 Influence of Rotational Effects of Natural Convection Embedded by Jeffrey Nanofluid Sheet in High Porosity

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Abstract

This paper deals with the influence of rotational effects of natural convection embedded by nanofluid layer in porous medium. The behavior of nanofluid is described by Jeffrey fluid model. The employed model incorporates the effects of Brownian motion and thermophoresis. The momentum-balance equation is modified due to the presence of Jeffrey parameter and nanoparticles. The stress-free boundaries are used here. The Eigenvalue problem is solved analytically as well numerically using Normal mode analysis and Galerkin Weighted Residuals Method (GWRM). Mathematica version 12.0 is used to calculate the values. The effects of the Jeffrey parameter, rotational parameter, Lewis parameter, modified diffusivity ratio, Nanoparticles' Rayleigh number and medium porosity are discussed analytically and numerically. Outcomes are also presented graphically.

Keywords: Convection, Nanofluid, Brownian Motion, Galerkin Weighted Residuals Method, and Porosity.

Synthesis, characterization of Sodium Niobate based Glass-**Ceramics for Energy applications**

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Abstract

Glass-ceramic material based on sodium niobate in silica glass matrix doped with Eu³⁺ was synthesized by melt quenching process followed by controlled heat treatment. The activation energy for crystallization of glassceramic was evaluated by Kissinger, Ozawa and Augis-Bennet model. Activation energies were noted to be about 260.569kJ/mole, 279.37 kJ/moleand 269.98 kJ/mole respectively. Ceramization of glass was carried at by double-stage heat-treatment at 650°C for nucleation and crystal growth at varying temperatures of 700°C and 800°C for 5 h. Crystal phase developed through ceramization was identified by XRD analysis followed by chemical bonding analysis through FTIR. Intensive chemical bonding analysis was carried by Raman spectroscopy. Refractive Index was evaluated using a Prism Coupler refractometer. Transmission spectra were evaluated using UV-VIS-NIR spectra while band gap was evaluated using Tauc plot. For base glass band gap was noted to be 3.502eV while after crystallization by ceramization heat-treatment band gap was reduced to 1.623eV respectively. PL spectra of the glass-ceramic sample also studied to note emission behaviour after excitation of samples at 395nm using Xenon lamp.

Keywords: Glass-Ceramics; Activation energy; Kinetic Model; Phase analysis; Bonding analysis; Band gap & PL.

Quantum Dot Based Fluorescent Biosensing Device for early screening and detection of cancer biomarkers

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Abstract

The present invention relates to an optical biosensing device for cancer biomarker detection using functionalized carbon quantum dots (CQDs) based fluorescent probe. More particularly, the intensity decreases because of dequenching of functionalized CQDs bioconjugate in presence of cancer antigen. The mechanism of detection is based on fluorescence turn "ON" and turn "OFF" mechanism in absence and presence of cancer antigen respectively. The proposed device is a prototype for Cancer detection at early stages. The portable fluorescent biosensor for cancer detection has easily portable and suitable for usages in labs and fields sites. Considering that it costs about INR 500, it is less expensive than other commercial biosensors. Very small sample volume— up to 0.5-10 μ L is needed to handle cancer samples. The device operated by electricity that allows experimental outcomes to be easily seen through visual detection. The portable device can be used for mass screening of women, where the presence of biomarker can screen women at very early stages, and hence can help is disease management and bringing down percentage of cancer related deaths of women in India. The process has already applied for Indian Patent and the design patent has been granted recently.

Keywords: Biosensor; Cancer detection; Diagnostics; Fluorescence; Optical; Quantum dots.

ICRTMD-2023/FIT/SIT/252 Synthesis of Hydrogel Nanocomposites by Radiation Assistance for Biomedical Applications

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Abstract

Biomaterials are any substance or combination of substances of synthetic or natural origin which treats, augments, or replaces any tissue, organ, or function of the body. Among different biomaterials, hydrogel are one of the potential candidates as they can mimic the physical, chemical, electrical, and biological properties of most biological tissues. Basically hydrogels are three dimensional hydrophilic polymeric networks which do not dissolve but can swell in water and retain the water within its network even under pressure. They possess excellent biocompatibility with blood, body fluids and tissues. Radiation assisted crosslinking of polymeric materials using ultraviolet (UV) rays, gamma rays, X-rays, and electron beam has been recognized and demonstrated on a large scale by many researchers. Radiation synthesis of hydrogels are considered to be clean and safe for human beings due to its non-involvement of crosslinking agents/other additives during the synthesis process. In the present work, synthesis of Ag/PVA, Au/PVA, and ZnO/PVA hydrogel nanocomposites was carried out using gamma irradiation technique. The physical and morphological characterization of the prepared samples were carried out using powder X-ray diffraction (XRD) and Field Emission Scanning Electron Microscopy (FESEM). The swelling studies were carried out understand the equilibrium degree of swelling (%EDS), swelling degree (%S), and swelling mechanism of the prepared samples. The prepared samples were also evaluated for antibacterial and cytotoxicity evaluation. It is been found that the prepared samples possess good antibacterial activity against gram positive and gram negative bacteria. The in vitro cytotoxicity studies showed that the prepared samples were non-toxic to human skin cell lines of diverse morphology. The unique advantages of radiation technology is been successfully utilized for the preparation of new products, with designed functions that satisfy expectations of patients and physicians.

Keywords: Hydrogel; Gamma Irradiation; Nanocomposites; Biomaterial; Radiation.

Behaviour of Cementitious Systems on Additions of Nano Silica

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Abstract

Cement, concrete, soil, sand, fly ash etc. almost all building materials have silica content i.e. they are siliceous in nature having high to very high silica content. Silicon Di-Oxide, SiO2 called Silica, in common parlance is one of the most stable materials which are ideal for construction use. Work presented by many authors reveals that the Silica Fumes improve the performance of cement composites & concretes through pozzolonic reactions but Nano-Silica additions have brought in further improvements in the mechanical properties & other properties of cement mortar due to nucleation and pore filling effects. This paper aims to investigate and analyze the mechanical performance for both blended & ordinary cements and the corresponding microstructures of Nano silica additions in ordinary cement composites. Micro structural SEM-EDS investigational studies indicate the presence of more hydrated products in Nano silica added cement composites, which is the reason for its strength gain.

Keywords: Cement, Nano-Silica, Optimization, Strength.

Influence of size and composition on fluorescence properties of carbonaceous nanoparticles (CNPs)

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Abstract

Carbonaceous nanoparticles (CNPs) are biocompatible, non-toxic, water soluble, photochemically stable and easy to functionalize materials which display optical properties suitable for a wide range of applications. However, they exhibit perplexing fluorescence properties which depend on factors like method of preparation, size, composition, etc. I will discuss the fluorescence properties of CNPs synthesized by hydrothermal method using glucose as a precursor and urea and sodium hydroxide as additives. The synthesized CNPs contain C, H, O and N, thus appropriately referred as carbonaceous nanoparticles. Two different compositions of CNPs were obtained. The fluorescence emission profiles for CNPs containing C, H, N, and O show an excitation wavelength dependent emission and lifetime decay fit to a bi-exponential function. The fluorescence quantum yield was found low for smaller size of CNPs. The results indicate that composition of CNPs dominate the fluorescence quantum yield of CNPs. The sizes of CNPs synthesized in present work were large enough for quantum confinement effects not to influence fluorescence emission properties. The second harmonic light scattering (SHLS) experiments were carried out to investigate nonlinear optical properties of CNPs. A strong broad multiphoton fluorescence is noticed along with the SH signal. The results obtained thus far will be presented and rationalized. Results describing the linear fluorescence properties of the synthesized CNPs are published in Journal of Photochemistry and Photobiology, A: Chemistry (Citation: Journal of Photochemistry & Photobiology, A: Chemistry 437 (2023) 114485).

Ecofriendly and sustainiable nanomaterials for the removal of hazardous contaminants from wastewater

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Abstract

The prolonged presence of antibiotic residues in the environment is caused by the widespread use of antibiotics to treat bacterial infections and day to day development of new antibacterial compounds for medication. Among various antibiotic residues, Doxycycline (DC) is a broad-spectrum antibiotic drug (tetracycline-class), highly consumed as it targets both gram-negative and gram-positive bacteria, thus can be used in the treatment of numerous diseases including prostate cancer, meningococcal bacteremia, lymphatic malformations and periodontal disease. After consumption, a huge percentage (50-80 %) of DC is excreted out as such via urine and faeces and goes directly into the surface water and groundwater. Additionally, the disposal of contaminated wastewater in the environment from hospitals and pharmaceutical industries is another major source of DC in the environment.

Facile green synthesis of nanomaterials such as CeO_2 -nps is an economic, easy, chemical-free and sustainable method. The synthesized CeO_2 -nps were found to be a promising photocatalyst for pharmaceutical residues degradation. The high photocatalytic efficiency (98.2%), rapid removal rate (30 min), great reusability (up to 5-cycles), and low-costs (USD 24.22) make the material exhibited its suitability towards water remediation.

Keywords: Nanomaterials; wastewater; antibiotics ; ecofriendly method.

Synthesis of Silver and Gold Nanoparticles using Syzygium samarangense Fruit Extract as Reducing Agent

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Abstract

Owing to their size-dependent optical, electrical and catalytic properties, noble metal nanoparticles especially of silver (AgNPs) and gold (AuNPs) have found applications in fields like electronics, optics, catalysis, biosensing, bioimaging etc. This study describes the simple, cost-effective as well as eco-friendly method for the synthesis of both AgNPs and AuNPs at room temperature by reducing 1 mM aqueous solution of silver nitrate and gold chloride with Syzygium samarangense fruit extract. Formation of AgNPs was found to vary with the synthesis temperature where as the formation of AuNPs was found to be spontaneous at room temperature itself. The yellow coloured AgNP colloid exhibited characteristic surface plasmon resonance (SPR) at 450 nm. The purple coloured AuNP colloid exhibited SPR at 541 nm. Crystalline nature of AgNPs and AuNPs was observed by the presence of peak at $2\theta = 380$ corresponding to (111) lattice plane in the X-ray diffractogram. The morphology of both AgNPs and AuNPs was studied using micrographs taken using Field Emission Scanning Electron Microscopy (FESEM). The elemental composition of synthesized AgNPs and AuNPs was investigated using the model reduction reaction of 4-nitrophenol to 4-aminophenol in the presence of strong reducing agent.

Keywords: 4-nitrophenol; AgNPs; AuNPs; FESEM; catalytic activity; Syzygium samarangense.
Advancements in Electrode Materials for Lithium-Ion Batteries: A Comprehensive Study

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Abstract

This study conducted electrochemical lithium insertion investigations on WNb₁₂O₃₃, synthesized by solid-state reaction (SSR) and sol-gel (SG) techniques, within the voltage range of 1.0-3.2V. The SSR-synthesized material exhibited a specific capacity of 221mAh/g with 15.6 Li inserted during the initial discharge. The SG method enhanced the rate capability and cycling properties, resulting in superior electrochemical cycling performance, particularly at high 'C' rates. The SG-synthesized sample displayed a remarkable specific capacity of 142mAh/g after 20 cycles at a 20C rate. TiNb₂O₇ and TiTa₂O₇ phases, synthesized using the solid-state reaction method, were investigated for electrochemical Li insertion/extraction, revealing stable structures and first-cycle discharge capacity values of 307mAh/g and 215mAh/g, respectively, within the voltage range of 3.0– 1.0V. After 20 cycles, TiNb₂O₇ and TiTa₂O₇ exhibited discharge capacities of 212mAh/g and 100mAh/g, respectively. Novel electrode materials, $W_9Nb_8O_{47}$ and $W_7Nb_4O_{31}$ phases, were successfully synthesized via a superficial sol-gel method, demonstrating ReO₃-type structures and redox couples of tungsten and niobium. The first cycle discharge capacity values for W₉Nb₈O₄₇ and W₇Nb₄O₃₁ phases were 197mAh/g and 227mAh/g, respectively, within the voltage range of 3.2–1.0 V. FeVMoO₇ and CrVMoO₇ phases, synthesized for the first time through a facile sol-gel method, exhibited three-dimensional structures and promising cathode properties for lithium-ion batteries. The first cycle discharge capacity values for $FeVMoO_7$ and $CrVMoO_7$ were 284 mAh/g and 264 mAh/g, respectively, in the voltage range of 3.2–1.5V. However, FeVMoO₇ showed a discharge capacity of 160 mAh/g after 20 cycles. Additionally, nanometer and micrometer-sized samples of FeNbO₄ were prepared using solgel polymeric precursor and solid-state reaction methods. Electrochemical lithium insertion studies indicated that the micrometer-sized samples exhibited insertion of 0.3 Li during discharge to 1.0V, while the nanostructured sample displayed insertion of 3Li/FeNbO₄ and extraction of 2.2Li during the first discharge and charge cycles. A reversible capacity of 120 mA h/g was observed after 20 cycles for the nanostructured FeNbO₄ sample. These findings collectively contribute to the understanding and developing of advanced electrode materials for lithium-ion batteries with enhanced electrochemical performance.

Keywords: Li-ion batteries, Cathode materials, Electrode materials, Cell performance.

Magnetoplasmon Core shell Nanostructure

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Abstract

A new structure composed of ferromagnetic material iron being a core and a reactive metal Aluminum being a shell is proposed for plasmonic-based sensor application. The RIS has been evaluated for Fe-Al core-shell nanostructure. It has been observed that sensitivity gets enhanced even at a smaller size. The sensitivity goes to 190 nm/RIU. The obtained results successfully demonstrate its strong potential applications in RI sensing and SERS. The study indicates superior scattering efficiency and sensitivity of nitrides, which is further augmented by better tunability. The optical properties of Al and Fe are analyzed by the Finite Difference Time Domain (FDTD) method for nanospheres and core-shell nanostructure. The variation in LSPR resonance peaks and refractive index sensitivity (RIS) are evaluated by varying the size of the nanostructure and refractive index of the medium. Aluminum nanospheres showed an LSPR value at 151 nm which is under deep UV region while a redshift and enhancement in RIS has been observed for Fe-Al core-shell nanostructure. This configuration works efficiently for the application in sensors and achieves a higher value of refractive index sensitivity.

Keywords: Plasmonic, Magnetic, Core shell, FDTD, Sensor

Band-gap Engineering of Nanostructured CdSe-Cu₂Se Thin Films

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Abstract

Nanocomposites of n-type CdSe and p-type Cu_2Se semiconductors are of importance for optoelectronic devices applications including photovoltaics and solar cells. We report the deposition of CdSe-Cu₂Se nanostructured thin films and study of their optical and electrical properties. We have chosen Cu₂Se as a dopant in CdSe because doping by Cu₂Se can tune the band gap of CdSe and can modify its optical response.

CdSe-Cu₂Se nanostructured thin films were deposited on glass substrates by thermal evaporation of CdSe and Cu₂Se powders for different weight% (wt%) of Cu₂Se. From the XRD results it was inferred that in addition to the incorporation of Cu₂Se into the CdSe lattice as substitutional doping for small wt% of Cu₂Se, Cu₂Se exists as a separate phase for large wt% of Cu₂Se in the samples. The particles seen in the AFM images showed clear decrease in size with increase in the Cu₂Se wt %. Micro-Raman and UV-Vis spectroscopy were used for the optical characterization of the samples. X-ray photoelectron spectroscopy was used to obtained information regarding the oxidation states of Cd, Cu and Se in the samples. The absence of satellite peaks of Cu²⁺ ruled out the possibility for copper in Cu(II) oxidation state. Electrical conductivity of the samples was measured at different temperatures to study the charge transfer mechanism through the films. The activation energy obtained from electrical conductivity measurements decreased with increase in the wt% of Cu₂Se. The photocurrent in the CdSe- Cu₂Se nanostructured films increased with increase in the wt % of Cu₂Se.

Keywords: Nanocomposites; Nanostructured thin films; Electrical conductivity; Activation Energy; Photocurrent.

Moving from Pb to Pb- Free Piezoceramics: A Review

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Abstract

Piezoceramic devices play a very important role in various industrial and research applications as sensors/ transducers/actuators, etc. The most commonly used piezoceramics today are Pbcontaining material. Due to their high piezoelectric properties and the possibility of their application-adapted shaping, ease of fabrication, etc., piezoelectric ceramics, based on Pbcontaining perovskites, are chosen as the active material for most of the piezoelectric applications. However, it is well known that lead is toxic as it deposits in various parts of the body leading to severe diseases. Researchers are working since 1990 to replace lead zirconate titanate (PZT) that contains in excess of lead. So current research is on developing new Pb-free piezoelectric materials with enhanced piezoelectric properties. In this contest a review article focussing on a comparative study of Pb contained and Pb-free systems would be helpful in finding new Pb-free material. Here, some Pb- free piezoelectric materials such as Barium titanate (BaTiO3; BT), potassium sodium niobate ((K, Na) NbO₃; KNN), bismuth sodium titnate ((Bi₁/2Na_{1/2}) TiO₃; BNT), Bismuth potassium titanate ((Bi_{1/2} K_{1/2})TiO₃; BKT) and Ba (ZrTi)O₃-(BaCa)TiO₃ (BZT-BCT) are studied and a comparative analysis of the electromechanical parameters of Pb containing and Pb- free materials are explained.

Keywords: Piezoceramics; Lead zirconate titanate (PZT); Barium titanate (BT); Potassium sodium niobate (KNN); Pb- free.

Design principles for materials with extreme Lattice Thermal Conductivity

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Abstract

The present work offers a comprehensive analysis of atomic mass and its impact on the phonon transport characteristics of Alkali Halides (AH's) utilizing first principles calculations. It has been observed that low-lying optical phonons have a substantial role in enhancing phonon transport and increasing thermal conductivity (kL) in materials with a mass ratio near to unity, in addition to their average atomic mass. Materials having a mass ratio near to unity have very low scattering rates, which leads to long phonon lifetimes. As a result, these materials exhibit an unusually high thermal conductivity (kL) within a certain series. The phonon lifetimes heavily influence the trends in kL, as shown by the tensile lattice strain-dependent phonon transport characteristics of BaTe and MgTe. In determining the anomalous trends in kL for AH's with a mass ratio approaching unity, phonon scattering rates (which are the inverse of phonon lifetimes) are more significant than phonon group velocities. Additionally, this research demonstrates that materials can be engineered to possess both high and low kL values through atomic mass manipulation. This opens up intriguing possibilities for the tuning of thermal conductivity in a wide range of applications.

Keywords: Lattice thermal conductivity, TDEP, Molecular Dynamics simulations, Phonon Transport.

ICRTMD-2023/FIT/SIT/274 Detection and Degradation of Pharmaceutical waste using Bismuth Sulphide Nanoparticles incorporated reduced graphene oxide/Silver substrate

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Abstract

Bismuth sulfide nanoparticles (BiS NPs), were synthesized via the hydrothermal method, and the reduced graphene oxide(rGO), and silver nanoparticles (Ag) were prepared using the chemical reduction method, and this rGO/Ag composite acts as a substrate. The synthesized nanoparticles are subjected to characterizations such as X-ray diffraction(XRD), scanning electron microscope(SEM), UV-Vis-spectroscopy, and photoluminescence spectroscopy. Commercially available paracetamol-500mg (PAM) and aspirin-300mg (ASP) were selected for photodegradation under visible light using the as-prepared composites in an aqueous solution. Photoluminescence spectroscopy is used to detect PAM and ASP, using the photo-excited electron transfer (PET) process, the limit of detection(LOD) obtained for PAM(8.70ppm) and ASP(4.43ppm) with a sensitivity of 0.9954 and 0.8002. Fourier transform infra-red spectroscopy(FTIR) was used to analyze the before and after degradation products, to confirm the disintegrated products obtained using photodegradation such as –COOH and – CH- using photo-induced electron-hole pairs.

Synthesis, characterization and biocompatability of macroporous polyhydroxyethylmethacrylate based cryogel

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Abstract

Supermacroporous cryogel materials are widely used in several areas such as chromatography, support for enzyme immobilization and catalysts, scaffold for growth of mammalian cells, sensors, and drug delivery. The studies on the formation of cryogels, i.e. the mechanism of cryotropic gelation started on late 70s. Subsequent research led to wide range of applications of cryogels in biotechnology. Cryogel matrices were proved to be biocompatible and the most preferable matrices for cell proliferation. In this study, we have prepared a gelatin immobilized polyhydroxyethylmethacrylate based cryogel material via two different chemical strategies. The material was characterized for its porosity (mercury intrusion porosimetry and scanning electron microscope) and permeability. Gelatin immobilization on cryogel was confirmed using bichinchoninic acid assay. The gelatin immobilized cryogel matrix was tested for its biocompatibility (in vitro) and growth of hybridoma clone producing monoclonal antibodies. The characterization studies of the cryogel matrix revealed that the scaffolds are supermacroporous, biocompatible, and capable of cell proliferation.

Keywords: Supermacroporous cryogels; Hydroxy ethyl methacrylate; N.N' Methylene bisacrylamide; Allyl glycidyl ether; ELISA, Biocompatible.

Structural analysis of Ag nanoparticles deposited on Si wafer and their influence on Si nanowire-based Gas Sensor

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Abstract

Here, the room temperature deposition of silver (Ag) nanoparticles (NPs) on silicon (Si) substrate has been carried out by a simple chemical route to investigate their elastic and micro-structural properties. The theoretical X-ray peak profile analysis has been pursued through the Scherrer model, modified Scherrer model, modified Williamson-Hall model, size-strain plot model and Halder-Wagner model. The X-ray diffraction (XRD) analysis results in the crystalline nature of Ag NPs having nearer dodecahedron structure. The parameters including micro-strain, internal stress and energy density have been estimated for all reflection peaks of XRD. The findings show that the nano crystalline size (NCS) estimated from all models is in reasonably good agreement. This analysis can pave the way for novel research avenues by comparing the estimated elastic and micro-structural properties of Ag NPs as a potential alternative tool to existing characterization techniques and helpful in fabricating different sizes of Ag-Si nanostructure-based gas sensing devices. The influence of Ag nanoparticles on Si nanowire towards acetone gas sensor has been studied and achieved remarkable sensitivity 98.77% at 5 MHz frequency with operating temperature at 50 °C.

Keywords: XRD, silver nanoparticles, nano-crystalline size, reducing gases, gas sensor.

Tin oxide thin films on Ag(111) : thickness and temperature dependent study

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Abstract

Growth and structure of tin oxide films on Ag(111) from submonolayer to thick film coverages up to 10 monolayer equivalent thickness have been studied using low energy electron diffraction (LEED), x-ray photoemission spectroscopy and angle-resolved photoemission spectroscopy techniques for both room temperature (RT) and high temperature (HT) (573 K). For RT growth, most of the tin is oxidised to form tin oxide (SnOx) as confirmed by XPS where no metallic component is seen. However, the grown films are not epitaxial or ordered which can be confirmed by no spots in LEED for higher coverage. Three oxidation states of Sn are noticed for HT growth, two of which are from oxide phase and another from metallic phase of tin with the surface is mainly composed of SnO2. LEED pattern shows the presence of $c(2\times 2)$ and (3×1) along with two different hexagonal multidomain type pattern.

Keywords: Photoemission spectroscopy, Oxides, Thin film growth, Low energy electron diffraction.

Bacterial Nanocellulose in Synergy with Herbal Extracts: Production and Characterization

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Abstract

Herbal extracts as traditional medicine has received a lot of interest in the current scientific environment. Herbs and their essential oils have long been known for their antimicrobial properties. Herbal medications are thought to be more effective against current and new antimicrobial drug-resistant infections. As a result, an in-depth evaluation of herbal-modified products is obligatory. This study shows the modification of low-cost bacterial nanocellulose with herbal extracts from medicinal plants to create "all-natural" antibacterial films. The BNC was synthesized here using a low-cost black tea medium which was left over after brewing a tea. The dipping method using bio-extracts of Tinospora cordifolia (giloy), Azadirachta indica (neem), and Terminalia arjuna (arjuna) was used to modify the synthesized BNC. FTIR, FESEM, and XRD were used to investigate the modified BNC. The modified BNC was tested with antibacterial activity against E. coli and A. viridans. T. arjuna-modified BNC demonstrated the most potent antibacterial action against E. coli and A. viridans, with inhibition zones of 27.04 mm and 27.41 mm, respectively, followed by Neem and Giloy. The moisture content and porosity values of BNC films validate their extremely hydrophilic nature and pertinency for a variety of biomedical applications such as antibacterial herbal biomasks, wound healing and as scaffold material in tissue engineering.

Keywords: Low-Cost Bacterial Nanocellulose; Herbal Extracts; Nanocomposites; All-Natural Antibacterial Films; Biomedical Applications.

ICRTMD-2023/FIT/SIT/281 Studies on preparation and physico-chemical characterization of green hydrogels

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Abstract

Xylan-rich hemicellulose based biodegradable nature of hydrogels is highly appreciable and core anticipation in the present scenario. Xylan-rich hemicelluloses can be copolymerized in producing green hydrogels for improving the absorption performance of many adsorbent products. Hydrogels are three-dimensional, crosslinked polymeric networks capable of absorbing and retaining both water and biological fluids and swell. When swelled, they are soft & rubbery and resemble the living tissue, exhibiting excellent biocompatibility. Crosslinking is one of the simplest reactions used to improve the physico-chemical properties of xylan-rich hemicelluloses which were extracted from corn cob by alkaline chemical treatment at room temperature. The hydrogels were prepared by free-radical graft co-polymerization reaction of xylan-rich hemicelluloses (which were dissolved properly in a mixture of solvent of 2-propanol and distilled water in 1:2 ratio) taken as a substrate with acrylic acid (AA) and acrylamide using N, N-methylene-bis-acrylamide (MBA) as a cross-linker in the presence of initiator potassium persulfate ($K_2S_2O_8$) system. Hydrogels were optimized on the basis of water holding capacity and mechanical strength. The optimized hydrogels was hold water upto 68g/g or 6800% when it was prepared by taking AA and xylan-rich hemicelluloses in the ratio of 2:1. Structural characterization was performed by using FTIR spectroscopy. The result ensures that the characteristic of prepared hydrogel are expected to play a crucial role in shaping the future of materials science and biomedical applications. The ability to imitate the natural environment of living tissues makes them ideal candidates for applications requiring controlled release of therapeutic agents in near future.

Keywords: Xylan; acrylic acid (AA); pH-responsive hydrogel; free radical polymerization.

ICRTMD-2023/FIT/SIT/282 Revolutionizing Therapeutics: Challenges and Innovative Solutions in 3D Printing

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Abstract

The convergence of 3D printing technology and personalized medicine has captured significant attention within the pharmaceutical and healthcare industries. This comprehensive chapter delves into the realm of 3D printing, with a specific focus on its applications in drug delivery and pharmaceutical product development. It extensively explores various types of 3D printers, such as inkjet, extrusion, and laser-based systems, and their diverse utilities in the field of drug delivery. The detailed review also sheds light on recent advancements in pharmaceutical 3D printing, particularly concerning drug delivery methods. However, it candidly acknowledges the existing technical and regulatory hurdles that currently hinder the widespread integration of this technology into the pharmaceutical and healthcare sectors. To address these obstacles, it puts forth potential solutions and strategies aimed at overcoming the challenges and paving the way for the successful adoption of 3D printing in these critical fields.

Keywords: 3D printing technology; Recent Advancements; Technical hurdles; Critical fields; Regulatory hurdles.

Synthesis, Electrochemical and Antimicrobial Studies of Ni(II) Complexes with New Macro Cyclic Schiff Base Ligands

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Abstract

A series of Ni(II) complexes have been synthesized with new Schiff bases ligand and various amino acids contain amines in aqueous methanol solution. The newly synthesized Schiff bases and their Ni(II) complexes have been characterized by elemental analysis, magnetic susceptibility, thermal, conductance measurements, mass, IR, electronic, 1H,13C-NMR spectral and electrochemical techniques. These ligands act as tetradentate species and coordinate to the metal center through the different potential donor atoms such as N and O. The probable square planar structures have been assigned to these complexes. A typical cyclic voltammogram obtained in the potential range of -1.6 V to +1.6 V (Ag | AgCl) on GCE for $[Co_2(CMAIPA)(H_2O)_4]$ an irreversible oxidation peak at ~ 0.850 V and another quasireversible reduction peak at ~-1.250 V are observed. All the synthesized Schiff base ligands and Co(II) metal complexes have also been screened for their antimicrobial activities and metal complexes found to be more active than respective Schiff-base ligands.

Keywords: Orthophthalaldehyde; Schiff-bases; Co(II) complexes; spectral studies; Electrochemical studies and antimicrobial activity.

Exact Solution of Optical Pulses in Nonlinear Meta-materials

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Abstract

Now-a-days metamaterials have become very popular because of their numerous potential applications in the fields of sensing, trapping, and imaging as they can exhibit a strong localization and enhancement of fields. Nonlinear pulse propagation in optics has led to innumerable innovations in several fields, the most notable of which are fibre optics and surface dynamics. The study of optical solitons in meta-materials is a new and exciting field of research where numerous theoretical and experimental results have been demonstrated by several groups. Meta-materials have been a subject of intense theoretical and experimental investigations due to their wide range of potential applications from super-resolution to cloaking. However, they are artificially structured materials where both the electric and the magnetic responses can be obtained at any required frequency regime. Most meta-materials show linear response where the dielectric permittivity (ε) and the magnetic permeability (μ) do not depend on the electromagnetic field intensities. However, the nonlinear metamaterials can be designed by putting together an array of thin wires and split ring resonators (SRRs) into a nonlinear dielectric. There have been investigations of ultra-short pulse propagation in nonlinear NRM where a wide class of solutions for bright and dark solitons phase locked with the sources has been analyzed for distinct parameter ranges. In this article, the nonlinear pulse propagation has been analytically studied by solving the nonlinear Schrödinger's equation (NLSE) in bulk media exhibiting frequency dependent dielectric permittivity (ϵ) and magnetic permeability (μ). The exact solutions obtained are shown to be of trigonometric & localized types. The analytical and simulation based method has been further extended to investigate the intensity distribution in a nonlinear meta-material which behaves as a negative refractive medium (NRM), where both ε and μ are shown to be dispersive and negative in nature. It is seen that the peak of the intensity curve decreases with increase in frequency towards the magnetic plasma frequency. The stability of the solitonic solution has also been established.

Keywords: Meta-materials, NRM, NLSE, SRRs, Solitons.

ICRTMD-2023/FIT/SIT/286 Synthesis of Silver Nanoparticles using Plumeria plant and its Larvicidal Activity against Malaria Vectors

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Abstract

Malaria is one of the longest known diseases in humans. Malaria is a serious public health problem due to the high cost of living and loss of life. The vaccines are not available for the prevention or treatments on malaria, dengue like diseases. The concept of findings is, to prepare silver nanoparticles (Ag NPs) by using green methodology. We use plant latex for the synthesis of Ag Nps and that material is used to control the mosquito vector. The synthesized Ag NPs are used for larvicidal activity against the malaria vector anopheles stephensi & filariasis vector culex quinquefaciatus. The Ag NPs were characterized by fourier transform infrared spectroscopy (FT-IR), UV spectroscopy, XRD analysis, scanning electron microscopy (FE-SEM). Ag NPs are effectively synthesized from a silver nitrate solution through a simple green route using the plumeria plant latex. It has potential to be used as an ideal ecofriendly approach for the control of the mosquito.

Keywords: Ag NPs, Green Method, Ecofriendly and larvicidal activity.



ICRTMD-2023/FIT/SIT/288 Magnetic Characteristics of La_{0.7}Ca_{0.3}MnO₃: Insights into the effects of Ni and Co doping through magnetic Compton spectroscopy

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Abstract

La_{0.7}Ca_{0.3}Mn_{0.95}(Ni/Co)_{0.05}O₃ Magnetic Compton profiles (MCPs) were measured at SPring-8, Japan, from 8 to 250 K using high-energy inelastic scattering. To quantitatively analyze magnetic property amendments, temperature-dependent MCPs were decomposed into profiles for Mn, Ni/Co, and itinerant electrons. Decomposed profiles revealed ferromagnetic coupling between Mn-3d electrons and Ni/Co ions, while itinerant electrons displayed anti-ferromagnetic links with Mn-3d and Ni/Co-3d electrons. Integration with VSM data showed anti-ferromagnetic coupling between orbital and total spin moments. Variations in magnetic response in undoped and Ni/Co-doped perovskites were attributed to mixed valence states of Mn. This MCP dataset serves as a concise guide for understanding the origin and examining magnetic responses in such manganites.

Keywords: Magnetic Compton profiles; Manganites; Spin moment.

Recent progress in applications of superhydrophobic coatings and surfaces in various fields

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Abstract

In Recent years, Term Superhydrophobicity gains immense attention among researchers and various industries as superhydrophobic materials exhibit excellent properties like self cleaning, anti drag, anti corrosion, antifogging and many more. In the presented paper, some of the recent application of superhydrophobic coatings or surfaces has been reviewed such as anti corrosion; protection of cultural heritage, decomposition of environmental pollutants through superhydrophobic substance, self cleaning, protective coating for solar panels etc. Composite or materials revealing elevated hydrophobicity, tunable protection material, and color profile compatibility could save environment, financial loss of various industries like metal industry, countries artifacts, monuments, and architectural elements. Present study highlights the rising demand of superhydrophobic coatings and surfaces in various industries like paint, metal/ alloy, glass, polymer etc.

Keywords: Superhydrophobic surface, Metal/alloy, protection coating, self cleaning, cultural heritage.

Anisotropic nanostructure hybrids for the removal of organic contaminants

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Abstract

The environmental impact of industrial waste, particularly from sectors like leather, consumer goods, textiles, and pharmaceuticals, raises significant concerns due to the presence of organic dyes. Aquatic ecosystems face serious threats as these dyes seep into water bodies. A practical approach to address such contaminations involves utilizing diverse forms of carbon, along with anisotropic nanoparticles (NPs) and nanohybrids, known for their photocatalytic activity. Anisotropic nanohybrids with distinct physical, chemical, mechanical, thermal, and electrical properties along multiple axes have garnered considerable interest in water purification. This discussion specifically delves into metal oxides (e.g. TiO_2 , ZnO) based nanohybrids. The synthesis processes employed for their production, characterization methods, and their effectiveness in treating various organic dyes have been examined. Ongoing research in this domain focuses on fine-tuning the photocatalytic properties of carbon-based nanohybrids, exploring innovative synthesis techniques, and comprehending the mechanisms involved in dye degradation. The ultimate aim is to develop water treatment solutions that are both efficient and sustainable, thereby mitigating the adverse environmental impact of industrial pollution.

Keywords: Industrial waste; organic dyes; nanohybrids; photocatalytic activity; adsorption.

Low-Spin Iron(III) Complexes in Neutral, Monocation, and Monoanion Forms Stabilized by Azo-Appended Tridentate o Amidophenolate(2-) and o-Iminobenzosemiquinonate(1-) π Radical

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Abstract

The study of metal-coordinated radicals has gained immense interest from perspectives of bio-inorganic chemistry, especially as model systems of various biologically active metalloproteins involved in multifaceted redox reactions in the body. One conspicuous example of such a metalloprotein is Galactose Oxidase. In recent years considerable interest is also directed to the understanding of electronic structures of transition metal complexes with redox-active/non-innocent ligands, due to their wide-spread presence in biological systems. The redox level of a non-innocent ligand (or ligands), coordinated to transition metal ions, cannot be unambiguously described by the chemical formula alone. In fact, the physical oxidation state differs from the formal oxidation state if an open shell organic radical is coordinated to transition metal ions.¹⁻⁴ From both these perspectives we have initiated a program to synthesize and to determine the molecular and electronic structure of such metal coordinated radical complexes using non-innocent ligands. In this continuing attempt, we have used a series of spectroscopic and electrochemical techniques, and finally performed the electronic structural calculations using Density Functional Theory (DFT) at the B3LYP level and have attempted to assign the redox level of both the metal ion and the ligand. Specifically, we have synthesized non-innocent ligand system containing azoappended o amidophenolate functionality and iron transition metal complexes (Parent complex, it's one electron oxidized and one-electron reduced complex). In this presentation an overview of our activity in this field will be highlighted.

Keywords: Galactose Oxidase, Non-innocent Ligands, Density Functional Theory.

Advanced Characterization Techniques in Nanocarbon Materials: An Inclusive Review

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Abstract

Current advancements in nanostructured carbon-based materials have found widespread application across various domains. Before using these carbon-based nanomaterials in different fields, many important challenges to be overcome. Biocompatibility, toxicity, elasticity, hardness, durability, reactivity, and various properties to be tested. We may investigate characterization techniques commonly employed in carbon-based nanostructure materials science. The focus is on elucidating the principles, applications, and significance of Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM), X-ray Diffraction (XRD), Nuclear Magnetic Resonance (NMR), Mass Spectrometry (MS), Atomic Force Microscopy (AFM), and X-ray Photoelectron Spectroscopy (XPS). Each technique is explored in depth, discussing its working principles, instrumentation, sample preparation, and specific applications in materials characterization. Integrating these techniques offers a powerful approach to a holistic understanding of diverse materials' structure, composition, and properties.

Keywords: Carbon-based nanomaterials, Characterization, sample preparation, instrumentation, advanced technique.

Lithium Ion Transport Studies in PEO - PMMA Based Blend Polymer Electrolyte Systems

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Abstract

Poly(ethylene oxide) (PEO) – Poly(methylmethacrylate) (PMMA) based Blended Polymer Electrolyte Systems (BPES) were studied to understand its transport properties and ionic conductivity using Impedance Spectroscopy technique. The BPESs were prepared by mixing high molecular weight PEO6 (Mw = 1x106) and low molecular weight PEO5 (Mw = 1x105) with PMMA (Mw =1.5x105), keeping the lithium perchlorate (LiClO₄) salt concentration constant. The ionic conductivity and transport properties of these systems were studied in the temperature range 303K – 318K. The charge carrier density (n), ion mobility (μ) and diffusion coefficient (D) were estimated using Bandara and Mellander approach. The ionic conductivity and transport properties were found to increase with the inclusion of lower molecular weight PMMA and PEO₅ into PEO₆ matrix. The maximum charge carrier density, mobility, and diffusion coefficient were achieved for the composition, PEO6 (96 wt%)-PEO₅ (2wt%)/PMMA (2wt%) – LiClO₄, with highest ionic conductivity value of 1.89x10⁻⁴ Scm⁻¹ at 303K. All the transport parameters exhibited strong temperature dependence and found to increase with temperature.

Keywords: Polymer electrolytes, Ionic conductivity, transport parameter, Impedance spectra.

Natures of reflected waves generated due to incident qP/qSV waves at the stress-free surface of a micro-mechanically modeled PFRC half-space

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Abstract

Piezoelectric materials are a special type of "smart" materials used in several applications like ultrasonic detectors, microphones, oscillators, AFM probes, transformers, NDT, sensors, etc. After applying these materials in several engineering applications for many years, certain drawbacks came to light, such as low electrical output, brittle nature and stiffness, etc. These points motivate researchers to develop the micro-mechanics of composite materials by different analytical and numerical methods. One of the primary objectives of this work is to present the micro-mechanical models of piezoelectric fiber-reinforced composite (PFRC) materials using the analytical techniques of Strength of Materials and Rule of Mixtures. After theoretically establishing the model, some electro-mechanical properties of PFRC are graphically demonstrated, their advantages over monolithic piezoelectric materials are explained, and some potential applications in scientific and engineering fields are also discussed.

Another primary objective is to analyze wave reflection phenomenon at the stress-free/rigid surface of a PFRC half-space. Waves propagating through a medium carry significant information about it; thus, it is imperative to analyze them meticulously. Quasi-longitudinal (qP) and quasi-transverse (qSV) waves are considered to be incident at the stress-free/rigid surface of a PFRC half-space, and they generate reflected qP, qSV, and electroacoustic (EA) waves, whose propagation angles are graphically demonstrated and analyzed. The crux of this problem is solving the equation of motion, which is a family of coupled second-order partial differential equations. Using appropriate boundary conditions and different fundamental laws and methods of Applied Mathematics like Generalized Hooke's law, Gauss equation, Generalized Snell's law, Separation of Variables, Cardan's method, Strength of Materials, Rule 2 of Mixtures, etc., the closed-form expressions of amplitude/energy ratios of all reflected waves and interaction energy are obtained. The obtained expressions are shown to satisfy the universal Law of Conservation of Energy, which in turn validates the problem. The influences of incident angle and stress-free/rigid surfaces on amplitude/energy ratios are shown graphically and exclusively & exhaustively analyzed. The obtained outcomes may help enhance the performances of highly sensitive surface acoustic wave (SAW) devices such as amplifiers, oscillators, filters, bio-sensors, etc.

Keywords: Piezoelectric fiber-reinforced composite (PFRC); Quasi-longitudinal (qP) wave; Quasi-transverse (qSV) wave; Electroacoustic (EA) wave; Reflection; Stress-free; Rigid; Strength of Materials, Rule of Mixtures.

A Novel Approach for the Synthesis of Nano Pigments and Their Application in Polymer Matrix

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Abstract

The main objective of the present study is to study the interaction of non-biodegradable toxic dyes, Crystal Violet (CV) and Indigo Carmine (IC) with naturally occurring clay minerals ((Montmorillonite (Mt), Bentonite (Bent) and Verniculite (Vt)) and their organically modified forms (OMt, OBent and OVt) in batch extraction mode and to develop a novel methodology for the synthesis of the value added products, clay based nanopigments without creating second generation waste materials. During extraction of CV and IC, it was observed that the uptake of CV was more onto pristine Mt, Bent and Vt and the uptake of IC was more onto OMt, OBent and OVt. CV was found in the interlayer region of Mt and Bent as supported by XRD data and zeta potential values confirmed the presence of CV on their surface (-17.6mV to -9.42mV in case of Mt, -31.1mV to + 32.2mV in case of Bent) whereas in case of Vt and organo Mt, Bent, Vt, CV was found on the surface as supported by XRD and zeta potential values. The increase in the particle size of pristine clays and organo clays further confirmed the presence of CV on their surface. IC was found only on the surface of pristine clays and organo clays as there was no change in the interlayer spacing of pristine and organo Mt, Bent, Vt. The surface interaction of IC was further confirmed from zeta potential and particle size values.

After extraction of CV and IC from aqueous media, the intense violet (CV treated pristine and organo Mt, Bent and Vt) and blue (IC treated pristine and organo Mt, Bent and Vt) colored solid residues obtained (also known as clay based nano pigments). The nano pigments further used as colorant in Poly(methyl meth acrylate) (PMMA) polymer matrix to form transparent polymer films where nano pigments play dual role, act as reinforcement filler by enhancing their various physico-chemical properties and a coloring agent by providing attractive bright color to the polymer matrix.

Keywords: Crystal Violet, Indigo Carmine, Zeta potential, Nano pigments, Polymer.

ICRTMD-2023/FIT/SIT/306 Synthesis, Characterisation and Biological Activity Studies of Novel Series of Isomeric Pyridyl-Tetrazole Ligands and Bivalent Metal Complexes

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Abstract

A new series of bivalent metal complexes of the type M-L1-4 were prepared with biologically active isomeric pyridyl-tetrazole ligands such as N,N-dimethyl-2-[5-(pyridin-2-yl)-1H-tetrazol-1-yl]ethanamine (L1), N,N-dimethyl-2-[5-(pyridin-2-yl)-2H-tetrazol-1-yl]ethanamine (L2), 2-[5-(pyridin-2-yl)-1H-tetrazol-1-yl]ethanol (L3), 2-[5-(pyridin-2-yl)-2H-tetrazol-2-yl]ethanol (L4) and MCl₂.H₂O in 1:1 metal ligand ratio. These complexes were characterised by elemental analysis, UVVis, IR, 1H, 13CNMR and mass spectral studies. EPR spectra of 1-4 bivalent metal complexes are characteristic of square planar geometry, DNA binding studies were carried by UV-Vis absorption, viscosity and thermal denature studies revealed that each of these complexes are avid binders of calf thymus DNA. The nucleolytic cleavage activities of complexes were carried on double stranded pBR322 circular plasmid DNA by using a gel electrophoresis experiment under various conditions, where cleavage of DNA takes place by oxidative free radical mechanism (\cdot OH). In vitro anticancer activities of complexes revealed that the bivalent metalcomplexes exhibit comparable cytotoxic activity when compared to the standard drug cisplatin.

Keywords: Isomeric Pyridyl-tetrazole derivatives; Bivalent metals; DNA binding; cleavage; cytotoxic studies.

Wound healing and regeneration properties of novel biocompatible chitosan biopolymer scaffold

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Abstract

Wound healing and regeneration are the two major concerns observed in comorbidities such as diabetes. In addition, burn patient's wound healing process is also delayed. Although biomaterials have shown remarkable performance since inception. But their toxicity and complicated surgeries for removal of the implants is a concern. In this context, biodegradable and biocompatible scaffolds have played a significant role which are self-degradable over a short period of time and subsequent surgeries are not required. In the present study a biodegradable chitosan-based biopolymer was synthesized, and it was assessed for biological properties, swelling and absorption potential, drug delivery capacity and toxicity. The results demonstrated that it has excellent swelling and absorption potential, and slow drug release properties. In addition, it is proven as non-hemolytic material on human blood samples. It was observed that the prepared material does not interfere with the growth and morphology of Danio rerio fin (DrF) cell line cells exposed to 20-100 μ g/mL of the biopolymer concentrations. Moreover, wound healing assay conducted on Danio rerio fin cell line (DrF) cells exposed to the biopolymer demonstrates a regeneration of cells after 36 hours of exposure. Based on the above findings it was observed that the prepared materials can be used for further studies such as animal models application and randomized clinical trials (RCT).

Keywords: Wound healing, drug delivery, nanoformulation, biopolymer scaffolding, medical applications.

Preparation and characterization of NBR based composite of Polythiophene and Modified Carbon Black

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Abstract

In recent years scientist have studied effect of functionalized fillers in rubber matrix to improve the properties due to enhanced molecular interaction between the filler particles and the rubber chains. In this work polythiophene and concentrated acid functionalized carbon are used as fillers in NBR (Nitrile rubber). The effect of the fillers individually and synergistically on the properties of NBR composite has been studied. Concentrated acid functionalized graphite and Polythiophene is added to NBR at varying ratio with the aim of improving the physical, electrical and mechanical properties of rubber material. An optimum loading value of 20PHR functionalised carbon has been found to impart the best set of properties. Further the synergistic effect of adding Polythiophene along with the optimally loaded functionalized carbon composite has also been studied during this work with an aim to further enhance the conductivity of the elastomer. It has been found that addition of 20 PHR treated carbon itself reduces the electrical resistivity of NBR by 10-10hm meter, while further addition of polythiophene with the graphite material reduces the resistivity with increase in loading quantity without negatively affecting the other properties. However, the tensile strength values are marginally lower than the values obtained from conventional carbon black fillers.

Keywords: Nitrile rubber, carbon black, polythiophene, composite.

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Rice husk nano-catalyst for biodiesel production from microalgae using nanocatalytic transesterification process

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Abstract

This study explores the synthesis of nanocatalytic biodiesel from the microalgae T. indica, as biodiesel is one of the sustainable and unconventional source of energy. The impregnation approach was exploited in formulating the nanocatalyst from rice husk ash doped with sodium oxide and nickel oxide and the maximum catalytic activity was found for the RHA/Na₂O-20%/Ni-10% catalyst. The nanocatalyst is further characterized by powder X-ray diffraction method (XRD), scanning electron microscopy equipped with energy dispersive x-ray analyzer (SEM-EDX), thermogravimetric analyzer (TGA), BET surface area analysis, FT-IR. The optimized nanocatalyst (RHA/Na₂O-20%/Ni-10%) had the basic strength in the array of $15.0 < H_{<18.4}$ with the particle size of 40-60 nm and surface area of $26.491 \text{ m}^2/\text{g}$. The nanocatalyst has been chosen for performing the transesterification process of microalgae lipid with methanol. The study discloses that the maximum biodiesel yield of 92% was accomplished at optimum condition of transesterification process of microalgae lipid at 4wt.% of catalyst stocking with process time of 2 hr. at reaction temperature 65° C by utilizing 12:1 molar ratio of methanol to oil. The nanocatalyst was recovered and reutilized again for 5 cycles of reactions, with the last cycles yielding 70% biodiesel. The resulting properties and FAME yield of biodiesel is compared with EN standards of conventional diesel also.

Keywords: Rice husk, nanocatalyst, Transesterification, biodiesel, Fatty acid methyl esters.

ICRTMD-2023/FIT/SIT/314 Synergies of Synthesis: Recent Advances and Broader Significance in Chemistry

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Abstract

This abstract provides an overview of the current landscape of synthetic chemistry, highlighting recent advances, challenges, and the broader implications for various scientific disciplines. Synthetic chemistry stands at the forefront of scientific innovation, continually pushing the boundaries of what is possible in the creation of new molecules and materials. The paper begins by examining breakthroughs in synthetic methodologies, showcasing cutting-edge techniques that have revolutionized the field. Innovations in catalysis, asymmetric synthesis, and sustainable synthetic processes are explored, emphasizing their role in streamlining chemical synthesis and minimizing environmental impact. The advent of artificial intelligence and machine learning in synthetic chemistry is a focal point of this review, underscoring how computational methods are accelerating the design and optimization of novel compounds. The integration of data-driven approaches and automation into the synthesis workflow is transforming the way chemists conceptualize and execute experiments, leading to increased efficiency and success rates. Furthermore, the implications of synthetic chemistry extend beyond the laboratory, influencing diverse fields such as materials science, medicine, and nanotechnology. Challenges and ethical considerations associated with synthetic chemistry are also addressed, acknowledging the need for responsible innovation. The review concludes by envisioning the future trajectory of synthetic chemistry, emphasizing the interdisciplinary nature of ongoing research and its potential to shape the landscape of science and technology in the coming years.

Keywords: Artificial Intelligence, Asymmetric Synthesis, Machine Learning, Novel Compounds, Synthetic Chemistry.

Sensing of Fe3+ ions with Nitrogen-doped Graphene Quantum Dots functionalized with Au Nanoparticles through Photodetection Method

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Abstract

In the human body system, iron is one of the crucial metal ions, the dysfunction of which may be the reason for numerous diseases, such as anemia, Parkinson's illness, Alzheimer's disease, cancer, etc. So for healthy living, the detection of Fe^{3+} is highly desirable. Numerous studies on Fe^{3+} sensing have been reported in the literature. However, most of these are based on liquid phase detection, which faces various limitations in the detection process such as the solvent effect, low reparability, low reproducibility, etc. Here, a solid phase detection of Fe^{3+} ions is presented with the help of photodetection method with high accuracy. For the detection of Fe^{3+} ions, nitrogen doped graphene quantum dots, and gold nanoparticle heterostructure (N-GQD@Au) is implemented as a photodetector. N-GQD@Au is synthesized from gold salt by using N-GQDs as the reducing agent. Then N-GQD@Au based photodetector is excuted to measure the photocurrent in the presence of different concentrations of Fe^{3+} . With the increasing concentration of Fe^{3+} , photocurrent is observed to reduce under the laser excitation 405 nm with -4 V bias. The reason behind the reduction of photocurrent in the presence of the Fe^{3+} is the charge transfer from N-GQDs @Au to Fe^{3+} by the complex formation. Fig.1 shows the change of the photocurrent of N-GQD@Au in the presence of Fe^{3+} ions. This detection method is further exemplified for real-life samples.

Keywords: N-GQD@Au heterostructure, photodecetor, Fe³⁺ ion sensing in real sample.



Fig 1: Change in Photocurrent of NGQD@Au in the presence of Fe³⁺.

Low power Paper electronics based Wearable Radiation detector by Engineering Perovskite Halides

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Abstract

In recent past, the material like, Perovskite halides exhibit several interesting electronic & optical properties hence; there is considerable interest in exploring this emerging class of material. The attributes like high carrier mobility, long carrier diffusion lengths, and tunability of the band gap with suitable dopants make perovskite halides attractive materials for investigating the basic physics as well as other device applications. In this report it would be shown that a paper based flexible gamma ray detector can be made using hybrid halide perovskite methyl ammonium lead bromide (MAPB). The wearable paper based detector is solution processed and works at room temperature with large area operation ($\sim cm^2$). It detects the gamma ray by virtue of changing its resistance probes as direct detection of gamma ray and uses IDE (inter-digitated electrodes) for boosting current response. This detector shows a maximum calibrated sensitivity 5.26 μ C/Gy/cm² and reasonable mobility –life time product ($\mu\tau$) ~2 × 10⁻⁵ cm²/V for substrate like paper. The detector can be operable in a wide range of gamma photon energy between 100 KeV to 1100 KeV. This wearable detector shows high degree of sustenance under exposure to high dose of Gamma radiation and was tested for a cumulative dose of at least 1.6 KGy and shows a high shelf life at least of 9 months and fast response time of a few seconds. The detector has low power consumption which can operate down to 1 V (DC) bias with a detector current ~ 1 nA and hence fully compatible with low power paper electronics. The sensitivity increases with bias and shows saturation beyond 40V bias. Such low power wearable gamma radiation detector is expected to have application potential in areas like health care and point of use quick radiation detection. And have potential use of radiation dosimeter for personal as well as environmental monitoring of radiation doses as a complementary of existing TLD based dosimeter.

Keywords: Hybrid perovskite halide, radiation detector, paper electronics, flexible/ wearable detector.

Size Modification of Green Synthesized Silver Nanoparticles under UV exposure and Its Bacterial Resistance

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Abstract

Silver nanoparticles (AgNPs) were successfully synthesized from aqueous silk fibroin solution by using UVirradiation technique. Here the SF solution acts as stabilizer, and the effect UV-irradiation time influence the particle size and shape of the AgNPs. The UV-Visible studies evidence the strong surface plasmon resonance (SPR) band at 428 nm, which confirm the reduction of Ag+ to Ag° in the aqueous SF solution. Transmission electron microscope (TEM) images implies that the AgNPs are well dispersed in aqueous SF solution, increasing the irradiation time the large number of particles of grains with narrow size distribution agglomerates. The synthesized AgNPs structurally characterized by X-ray diffraction technique. The XRD pattern the peaks are good agreement with the synthesized AgNPs are face centered cubic structure (FCC) with a lattice constant of a = 0.485 nm. The dynamic light scattering (DLS) investigates the particle size distribution and average size of the synthesized AgNPs. The size control of AgNPs due to UV irradiation time can affect the significant antibacterial activity of SF-AgNPs composite, against four bacterial stains, i.e. Staphylococcus aureus & Bacillus subtilis (Gram positive) and Escherichia coli & salmonella typhi (Gram negative).

Keywords: Silver nanoparticle; Silk fibroin; UV-Visible; XRD; TEM; DLS; Antibacterial activity.

Synthesis, Characterization and Computational Investigation of 4-(4-bromophenyl)-2-(4-chlorophenyl)-2,3-dihydro-1H-benzo[b] [1,4] diazepine

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Abstract

This work deals with the synthesis of 4-(4-bromophenyl)-2-(4-chlorophenyl)-2,3-dihydro-1H-benzo[b] [1,4] diazepine by condensation of intermediate (E)-1-(4-bromophenyl)-3-(4-chlorophenyl)prop-2-en-1-one with the ortho phenylenediamine in alkaline medium. The structure of the synthesized compound was established by FTIR, 1H NMR, 13C NMR and HRMS spectral techniques. The density functional theory (DFT) calculations at the B3LYP level were performed for the synthesized compound employing the Gaussian 03(W) package. The optimized geometrical parameters, electronic parameters, frontier molecular energies, and global chemical reactivity descriptors have been determined at the DFT/B3LYP/6-311++G(d,p) level. The thermodynamic properties and the molecular electrostatic potential (MEP) were also examined using the same level of theory. Moreover, the vibrational wavenumbers of title compound were computed and the scaled results were compared to the experimental FT-IR spectra. The findings show a good correlation between computed and experimental frequencies.

Keywords: Diazepine, NMR, DFT, Gaussian, vibrational wavenumbers.

ICRTMD-2023/FIT/SIT/338 Synthesis and Characterization of Superparamagnetic NFO Nanoparticles using Hydrothermal Method

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Abstract

Hydrothermal method was used to synthesize Nickel ferrite (NFO) nanoparticles using two different reducing agent NaOH (T–series) and NaBH₄ (N–series). Effect of synthesis temperature on the structural and magnetic properties was studied using two different reducing agents, sodium tetrahydridoborate (NaBH4) and sodium hydroxide (NaOH). X–ray diffraction (XRD) and Raman spectra were used for the structural study. The single phase nanoparticles started to form at temperature 120°C and 160°C for NaBH₄ and NaOH as a reducing agent respectively. Also, the crystallite size of the nanoparticles calculated using XRD data was found to be in the range of (12–22 nm) in the case of the NaBH₄, while the samples prepared using NaOH has size in the range (35–40 nm). The increasing order in size from 12 nm to 22 nm has been observed with an increase in synthesis temperature for the N–series. SEM confirms the nano-octahedron morphology of NFO nanoparticles of T–series. The measurement of magnetic properties was complete at room temperature using the physical property measurement system (PPMS). A regular trend in crystallite size and coercivity was observed for the samples prepared using NaBH₄ as a reducing agent with temperature. It was found that nanoparticle behavior tends to superparamagnetic from ferromagnetic as we increase the synthesis temperature. But no regular magnetic behavior has been shown by the nanoparticles prepared using NaOH as a reducing agent.

Keywords: Nickel ferrite, Hydrothermal method, Temperature effects, reducing agent, superparamagnetic.

Designing of Flexible and Moldable Bamboo Fiber – Reinforced Brine Sludge PDMS Based Composites for Thermal Insulation Applications

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Abstract

The current scenario urges the utilization of renewable and biodegradable feedstock due to the inevitable depletion of fossil-based resources and their detrimental environmental hazards. Similarly, due to the recent unprecedented urbanization and industrialization, wastes and pollutants generated from these activities are badly affecting the environment. Herein, thus, an innovative method for utilising naturally available bamboo resource and chlor-alkali waste brine sludge embedded with polydimethylsiloxane (PDMS) is reported. The present investigation's goal is to present an intensely flexible, moldable and stretchable polymeric architecture consisting of bamboo fibre powder and brine sludge in PDMS matrix in various ratios as an effective thermal and mechanical active material. The thermal investigation is conducted using the developed flexible material at room temperature and the result shows that the developed flexible material offers thermal insulation properties. Further, field emission scanning electron microphotographs of the advanced flexible materials revealed pores in the matrix, which gives the material its insulating properties. The characterization study also reports tensile strength and compression capabilities of the developed material. Consequently, these flexible composite material developed based on bamboo-brine sludge has a variety of applications across an extensive selection of fields and can be an alternative in various applications especially thermal insulating applications.

Keywords: Bamboo fiber powder; Brine sludge; PDMS; Flexible; Moldable.

ICRTMD-2023/FIT/SIT/342 Mechanical study of Polymer composite reinforced with surface-modified Napier grass stem cellulose nanofibrils

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Abstract

In this research the Cellulose nanofibrils, a natural fiber is used as a reinforcement material and epoxy polymer as the matrix material. Cellulose nanofibrils (CNFs) prepared from Napier grass stems via alkalization, bleaching and sulfuric acid hydrolysis treatments. Varying percentage of this natural fiber is used for developing a unique composite. Tensile strength increased with increasing filler loading. The modulus and hardness of the composites are increased continuously with increasing filler loading. The proposed composite material satisfies recent trends, and they can be used as a potential replacement for the commonly used composites for aerospace applications.

Keywords: Epoxy Polymer; Cellulose nanofibrils; Napier grass Surface modification; Reinforcement; Mechanical properties.

ICRTMD-2023/FIT/SIT/350 Hierarchical Nano and Micro Scale Structures formed by Selfassembled MgO and ZnO Quantum Dots in Presence of LC Media

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Abstract

We have explored the effects of introducing ZnO and MgO nanoparticles into 4-(trans-4-nhexylcyclohexyl) isothiocyanatobenzoate. We conducted a thorough analysis of the dielectric properties, opto-electronic features, and calorimetric phase-transition characteristics of liquid crystal (LC) upon doping MgO and ZnO NPs. We carefully prepared a uniform mixture of MgO and ZnO NPs in toluene and transferred them into cells made of glass and Indium Tin-Oxide (ITO) coated glass. The resulting hybrid systems revealed distinct microstructures classified into three main categories: grain-like structures formed by smaller-sized MgO nanoparticles with liquid crystal molecules anchoring over their surfaces; these grain-like structures further combined to create inorganic polymeric honeycomb-like meso-structures in the presence of the glass surface; and flower-like clusters of MgO nanoparticle aggregates on the ITO surface. Smaller nanoparticles effectively maintained energy balance by facilitating the anchoring of liquid crystal molecules, while larger counterparts failed to achieve energy equilibrium, leading to the formation of more extensive nanoaggregates or clusters. The interaction between the substrate and nanoparticles surface energy preference for liquid crystal molecules played a crucial role in shaping diverse hierarchical nano- and microstructures. Our understanding of these structural formations is derived from the delicately balanced competition among various forces: NP-NP, LC-LC, NP-LC, Glass/ITONP, and Glass/ITO-LC interactions. Significant changes were observed in the dielectric properties, transition temperature, bandgap, and other parameters of LC molecules following MgO NP doping, while ZnO NP doping induced minor alterations. Using a theoretical model, we estimated the size and shape of the resulting nanoclusters in the liquid crystal medium. The trends in the size dependent bandgaps for MgO and ZnO NPs are found to be opposite. We account reasons for that. To elucidate the doping effect, we calculated changes in enthalpy and specific heat capacity for the LC-NP system. The confirmation and validation of our findings were conducted through various characterization techniques, including Optical Microscopy, FTIR, Raman, IR, HR-XRD, and FESEM - EDX analyses.

Keywords: Grain Structures, Flower-like micro-structures, Honeycomb-like Mesostructures, ZnO NPs, MgO NPs, Bruc model, Free energy minimization.
Investigation on SnO₂/graphene-based nanocomposites for supercapacitor application

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Abstract

Al doped SnO₂ nanoparticles and their rGO composites are prepared by co-precipitation and hydrothermal method respectively. PXRD analysis of prepared Al doped SnO₂ compounds show lower angle shift with increased peak broadening. Crystallite size of Al doped SnO₂ nanoparticles and its composites decrease from that of pure SnO₂. FTIR and Raman analysis confirms the tetragonal rutile phase for all synthesized samples with pronounced peak shift towards higher frequencies. FESEM images reveal Al doped SnO₂—rGO composites form stacked multilayers with aggregated particles on the sheets and irregular zigzag edges. From electrochemical analysis, integration of SnO₂ nanoparticles on 2D graphene enhances the specific capacitance values. Thus the insertion of appropriate amount of SnO₂ and graphene composition could provide a promising kind of electrode material for high-performance supercapacitors.

Keywords: SnO₂; graphene; nanocomposites; supercapacitor; electrochemical performance

Graphical Abstract:



Cyclic voltammogram of pure SnO2 and Al/SnO2-rGO composites

Unveiling the potential of two-dimensional V₂S₂ monolayer as a high-performance anode material for metal-ion batteries: A first-principles study

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Abstract

Using first principle calculation we have predicted for the first time that the V_2S_2 monolayer may be an efficient anode material for metal (Li, Na, K)-ion batteries. We have investigated the pristine V_2S_2 monolayer system's energetical, and thermal stability using first principle density functional theory (DFT) VASP code. The intrinsic metallicity of the pristine V_2S_2 monolayer facilitates its electrical conductivity as an electrode material. We also investigated the structural and electrical properties of the metal (Li, Na, K)-adsorbed V_2S_2 monolayer. It is observed that metal atoms prefer to get intercalated on top of the buckled hexagon of the pristine V_2S_2 monolayer, and the metallicity of the 2D nanosheet is preserved. Out of four possible adsorption sites namelyhollow site (h-site), vanadium site (V-site), sulfur site (S-site) and vanadium-sulfur site (V-S site), the hollow site is the most favorable one. In the hollow-site adsorption process, Bader charge analysis provides 0.99, 0.99, and 0.87 electronic charge transferred from the Metal (Li, Na, K) atom to the V_2S_2 monolayer. Furthermore, this system exhibits a high storage capacity of 968.9 mAh/g for both Li and Na and 322.9 mAh/g for K. This V_2S_2 system manifests moderately low diffusion energy barrier of 0.55 eV, 0.25V, and 0.27eV for Li, Na and K respectively. The calculated open-circuit voltage of 0.68 V, 0.71 V and 1.40 V for Li, Na and K respectively. Our results suggest that the V2S2 monolayer may be a potential candidate for anode material for rechargeable monovalent (Li, Na, K)-ion batteries.

Keywords: Metal-ion battery, Lithium ion battery, Sodium ion battery, first principle calculation, density functional theory.

Structural, Optical and Ionic conductivity Study of Copper Sulphide Quantum Dot Synthesized in Starch Matrix for Its Optoelectronic Device Applications

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Abstract

Copper sulphide quantum dots were synthesized by a simple chemical root. The XRD exhibited polycrystalline hexagonal structures of the synthesized quantum dots. There was an enhancement of quantum confinement with lowering molar concentration. The HRTEM showed spindle type particle distribution in large area. The UV-vis. spectroscopy showed a systematic blue shift of absorption with lowering molar concentration. The copper and sulphur sources capped with 3% of starch exhibited good physical properties viz. size of quantum dots compared to other capping materials. Starch supported the growth of uniform nanostructures and protected the quantum dots from agglomeration to a large extent. Amonia played important role in stabilizing the synthesized material well inside the matrix material. The tauc-plot estimation of optical band gap showed the enhancement of band gap from 1.9eV to 3.6eV confirming the good quantum confinement of the synthesized material. The photoluminescence (PL) spectroscopy also showed the same nature of blue shift of emission (UV-blue) with lowering molar concentration. The ionic conductivity study showed good semiconducting behavior. The synthesized material may be exploited in fabrication of UV-blue LED.

Keywords: Quantum dot; capping agents; low molarities; UV-blue emission; precursor materials.

Graphene the Wonder Material of 21st Century

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Abstract

Graphene, one of many allotropes of carbon, either a single layer of carbon atoms or several layers of this honeycomb structure piled up, has got the attention of engineers and scientists alike. The term graphene is a amalgamation of the word graphite, and the suffix -ene, referring to polycyclic aromatic hydrocarbons. Unlike bulk graphite, this 2-D material exults flexibility, strength, and most amazing electronic properties waiting to be exploited in range of applications. Starting from theoretical study of graphene by physicist Philip R. Wallace as a first step to investigate the electronic structure of graphite, to the 2004 isolation of single layer of graphene by "scotch tape method" by University of Manchester physicists Konstantin Novoselov and Andre Geim, Graphene mania peaked in 2010 when the material's discovery led to that year's Nobel Prize in Physics. Since that time, researchers across the world have been enchanted with thin films and have succeeded in preparing a wide variety of so-called two-dimensional materials beyond graphene loke phosphene, silicene etc. and graphene have become the front-runner for becoming the replacing silicon in near future. A number of experimental and theoretical studies have been performed on graphene in this regard. Our group performed Density functional Density calculations on graphene to analyse the geometry and electronic structure and optical properties of isomers of B, N, and BN doped graphene sheet. Through our detailed analysis, we suggest a theoretical method to design hetero- graphenes with different amount and composition of either B or N doping or co-doping of both (BN). Both mechanisms result in tuning of band gap in a wide range, for device applications. Due to their tunable band structure properties, the resulting materials can be used in applications in various sectors, e.g., nano electronics, gas sensing, hydrogen storage. A major red-shift in absorption spectra towards the visible range of the light at high doping concentration is reported for the B/N co-doping. The results open opportunities for application of graphene in photo electronics by modulating the optical properties of graphene in the visible region by the present method. The results provide motivation to do further work in this direction.

Keywords: Graphene, 2-D material, band-gap, electronic structure, optical properties.

ICRTMD-2023/FIT/SIT/362 Design and fabrication of 2D photonic crystals 1 employing electron beam lithography

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Abstract

The research aims to fabricate nano-scale features using non-dedicated EBL and capacitively coupled RIE for optical applications. Our empirical research methodology consists of three phases. The first phase consisted of gathering a suite of real benchmark circuits/devices and conducting statistical analyses of data sets to design a 2D photonic crystal (PhC) structure made of square/triangular lattice holes on silicon wafers with different dose factors. The second phase consisted of lithography using a beam of electrons to expose resist, an essential process for IC circuit fabrication and photonic crystals. During the third and final phase, the proposed work will design and perform experiments to study various photonic integrated circuits using electron beam lithography and the RIE etching tools. Moreover, the proposed work has constructed a complete EBL flow, which is created by augmenting and modifying various commercial and academic agencies, including chemical processing (RCA1, RCA2, Piranha), non-dedicated E beam lithography (Carl Zeiss Sigma 300 FESEM+ Raith Elphy Quantum lithography attachments) has been optimized for nanofabrication using the capacitively coupled reactive ion etching from the hind high vacuum.

Keywords: Silicon; photonic crystals (PhCs); FESEM Sigma 300; EBL; Nanofabrication.

ICRTMD-2023/FIT/SIT/364 Unlocking the Potential: Scandium-Doped ZnO Thin Films for Advanced Optical Limiting Applications

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Abstract

In this article, our primary focus is on elucidating the optical limiting behavior demonstrated by ZnO thin films, meticulously crafted using the sol-gel spin coating technique. The intrinsic characteristics of ZnO nanocomposites make them suitable for functioning as robust optical limiters across a broad spectral range, spanning from visible to infrared regions. Rigorous investigation into the nonlinear optical response of these intriguing nanocomposites has been carried out using nanosecond laser pulses operating at a wavelength of 532 nm. The exploration of the nonlinear optical properties of SZO thin films, with varying Scandium (Sc) concentrations, has yielded insightful findings. Particularly noteworthy is the peak value of nonlinear absorption coefficients observed in the SZO film doped with 0.6 atomic percent (at.%) of Scandium (Sc). This remarkable achievement can be unequivocally attributed to the exceptional crystalline quality exhibited by the sample with 0.6 at.% Sc, setting it apart from its counterparts. This outstanding parameter holds significant promise for the future, positioning SZO thin films as highly promising candidates for facilitating third harmonic generation, with substantial potential for advanced optical applications. Interestingly, an investigation into the optical limiting behavior reveals that the SZO film doped at a Sc concentration of 0.6 at. % boasts the most favorable limiting threshold. This distinctive metric serves as a clear indication of the material's impressive capability to effectively mitigate intense optical energy.

Keywords: Nonlinear Optics, ZnO, Thin Films, Optical Limiting, Transition Metal.

ICRTMD-2023/FIT/SIT/365 Next generation high-frequency rectifiers using spin-torque and nonlinear Hall effect

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Abstract

Due to the explosive growth of low-power portable wireless 5G (3.5-6 GHz and 24-86 GHz) technology in the smart cities, there is a great interest in developing micro-scaled high-frequency sensors and energy harvesters. Furthermore, many global cities are further expanding toward the future prospectus of 6G (95 GHz and above) and mm Wave (30-300 GHz) technologies for much faster (targeting 1Tb/s) and secured data transmission. This enables the critical need for the development of compact, highly sensitive broadband high-frequency rectifiers to be used in the next-generation sensor technologies. The wide-range applications of these high-frequency rectifiers are proposed in the fields of biomedical, telecommunication, meteorology, radars, etc. Existing high-frequency devices are mainly based on the semiconductor diodes, which suffer from the thermal threshold voltage, limited transit time, low frequencies, high junction-area, and high impedance. Furthermore, there is a so-called terahertz gap (0.1 to 10 THz) between the operating frequencies of electrical diodes and photodiodes. Instead of using semiconductor junctions, rectification can be realised by the nonlinear electrical or optical response of non-centrosymmetric topological materials (TMs) like Dirac/Weyl semimetals and topological insulators or resonant ferrimagnetic materials, with the final aim of integrating and scaling them in the commercial energy harvesting system or CMOS technology operating at microwave to mm wave frequencies.

Keywords: Spintronic and Topological Quantum Materials.

A paradox of pollution and purity of Ganga River in India

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Abstract

In India, the river Ganga is believed as a goddess, and people worship it. Despite all the respect for the river, the river's condition is worsening, and we Indians are unable to maintain the purity of the river. The Ganga is a river of faith, devotion, and worship. Indians accept its water as "holy," which is known for its "curative" properties. The river is not limited to these beliefs but is also a significant water source, working as the life-supporting system for Indians since ancient times. The Ganga river and its tributaries come from cold, Himalayanglacier-fed springs, which are pure and unpolluted. But when the river flows downgradient, it meets the highly populated cities before merging into the Bay of Bengal. From its origin to its fall, its water changes from crystal clear to trash-and sewage-infested sludge. Thousands of years passed since the river Ganga, and its tributaries provide substantial, divine, and cultural nourishment to millions of people living in the basin. Nowadays, with the increasing urbanization, the Ganges basin sustains more than 40 percent of the population. Due to the significant contribution of the growing population and rapid industrialization along its banks, river Ganga has reached an alarming pollution level.

Keywords: Ganga river; Water pollution; River pollution; Unethical practice; India.

Systematic Study on Material Selection

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Abstract

This article illustrates the significance of material selection in all aspects of engineering design. When choosing a material for a specific application based on its properties, appropriate testing must be executed in order to guarantee that the material will remain compatible with its intended application throughout the product's intended life. Tensile testing determines how something will react when it is pulled apart, or when a tension force is coupled to it. Tensile testing is one of the most basic and commonly used mechanical tests. The characteristics of a material can be assessed by determining the force required to expand a specimen to breaking point, allowing designers and quality managers to anticipate how materials and products will perform in the applications they were designed for. The choice of materials is based on maximizing performance of the material based on practical demands, geometry, and material attributes.

Keywords: material selection; tensile strength; strength; material attributes

ICRTMD-2023/FIT/SIT/372 In₂Se₃ and Bi₂Te₃ thin films based efficient TEGs for self-powering devices

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Abstract

A global demand of energy is increasing day by day and the sources of energy are still majorly depended upon the fossil fuels which leads to global warming and are decaying. This makes it very necessary to find other energy sources or save energy from where there is energy loss. Thermoelectric effect is one of the important way where the temperature difference can be directly converted into electrical energy which is an efficient method to harvest energy from the waste heat from industrial waste, heavy automotive vehicles etc. Thermoelectric materials have gained a great attention as a clean energy source to harvest energy from the waste heat to an electrical energy. In₂Se₃ have a low thermal conductivity and high electrical conductivity simultaneously and thus offers a good thermoelectric properties at room temperature. Also, bulk Bi2Te3 is wellknown to exhibit a high thermoelectric properties at room temperature, but is toxic and expensive. However, the thermoelectric properties of In₂Se₃ thin films are not been explored. Thin films offers a low thermal conductivity due to the presence of strong phonon scattering offering their application in the nanostructured devices. In the present work, the effect of post annealing on the thermoelectric properties of In₂Se₃ thin films are studied and compared with the performance of Bi₂Te₃ thin films, grown using thermal evaporation. The In₂Se₃ thin films annealed at 300 °C shows a high Seebeck coefficient calculated using an indigenously developed system. The thermal conductivity was calculated using 3ω -method which is found to be 0.75 Wm⁻¹K⁻¹ with a power factor and figure of merit of 12.04 μ Wm⁻¹K⁻² and 4.9 × 10⁻³, respectively which are found to be comparable with Bi₂Te₃, calculated at room temperature. These results indicate use of thermoelectric material thin films as an integrated power source for microelectronic device applications.

Highly efficient low temperature operated NO₂ gas sensors

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Abstract

Air pollution may be defined as any atmospheric condition in which certain substances are present in such concentrations that may produce undesirable effects on human beings and ecosystem. Nitrogen oxide (NO_2) is an important pollutant amongst other pollutants like SO₂, CO, CO₂ etc. Constantly increasing level of NO₂ gas is harmful to living beings as it is irritating to the upper respiratory tract and lungs even at low concentrations. Immediately Dangerous to Life or Health Concentrations (IDLHs) of NO₂ gas has been declared to be 20 ppm by Occupational Safety and Health Administration, USA. Thus, precise detection of trace level of NO₂ has become need of an hour. Hence, it is necessary to develop small size, highly sensitive and cost effective NO₂ gas sensors to detect low concentration of gas at lower operating temperature. Tin oxide (SnO₂) is the most preferred material for gas sensor application because it is sensitive to many gases and some degree of selectivity can be conferred by the use of appropriate additives. Efforts have been to study the effect of different modifiers (p-type or n-type metal oxide) incorporated with n-type SnO_2 thin film in enhancing the sensing response with reduction in operating temperature. To improve the response parameters of the sensor, different modifiers (WO₃, TeO₂, Al₂O₃, NiO, CuO, In₂O₃, ZnO, TiO₂, Ag₂O and PdO) in the form of microclusters have been deposited over SnO₂ surface. Origin of heterojunctions formed at the interface of different metal-oxide (p-type or n-type) modifiers and n-type SnO₂ thin film surface and its implication in enhancing the sensing response has been studied. Furthermore, efforts are also made to develop room temperature operated NO2 gas sensor by using hybrid nano-composite of multi-walled carbon nano-tubes (MWCNTs) and SnO₂ nanoparticles (NPs) nanostructures with varied concentration of MWCNTs. The sensor made using 5 mg of MWCNTs yielded a maximum response of about 1.07×10^3 at room temperature with fast response time (4 min) and recovery time (8 min) towards trace level (100 ppb) NO₂ gas. Also, to prepare handheld gas sensor based on SnO₂ film for onfield detection of NO₂ gas, effort has been made towards the miniaturization and packaging of complete sensor device.

Development of Metal Matrix Composites by Powder Metallurgy using Cold Isostatic Compaction Chamber: A Review

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Abstract

Metal matrix composites are being used in all scientific fields and are in high demand across a range of industries and applications. Therefore, improvements to the mechanical characteristics of metal matrix composites are crucial now. Due to wetting property, interface matrix, and agglomeration, manufacturing metal matrix composite using standard procedures presents a significant problem. Therefore, the ideal method for creating nano-composites is powder metallurgy with cold isostatic compaction. The benefit of this procedure is that it achieves a uniform distribution of reinforcement particles throughout the matrix and gets rid of any flaws such nanoparticle clustering. The major focus of this review study was on the value of powder metallurgy in achieving a uniform distribution of reinforcement in the matrix by utilising a cold compaction chamber.

Keywords: Metal matrix composites, Powder metallurgy, Nanoparticle, Cold isostatic compaction, Agglomeration.

Structural Stability and Ferromagnetism in Ga_{0.875}Cr_{0.125}P : DFT Study

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Abstract

The theoretical calculations of structural, electronic, and magnetic properties of $Ga_{0.875}Cr_{0.125}P$ Diluted Magnetic Semiconductor (DMS) in Zinc Blende phase (B3) have been performed using Density Functional Theory (DFT) as implemented in the Spanish Initiative for The Electronic Simulations with Thousands of Atoms (SIESTA) code with LDA+U (U=3) exchange-correlation (XC) potential. The study of spin polarized electronic band structures and magnetic properties represents induction of half metallic ferromagnetic behaviour in $Ga_{0.875}Cr_{0.125}P$ with 100% spin polarization. The hybridization of Cr-3d states with s and p states of Ga and P develops some local magnetic moment on non-magnetic Ga and P atoms. **Keywords:** DMS, GaP, ferromagnetism, DFT, Transition Metal, doping.

ICRTMD-2023/FIT/SIT/379 Silver Coated 1D Random Photonic Crystals for Sensing of Cancer Cell

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Abstract

In this paper, we have developed cancer cell sensor using the silver coated one dimensional random phonic crystal. Here, we achieved randomness through either a random layer layout or by randomly varying the thickness of the layers. Random photonic crystals were created using the dielectric materials silicon (Si) and silicon dioxide(SiO₂). Analytes are deposited in a random sequence in the sensing layer (SL), which is coated with silver (Ag) and sandwiched between the Si/SiO₂ layers. The unit cell of the photonic crystal as ratio of 1: 1 proportion of Si and SiO₂. For the construction, we employed 10 layers of Si, 10 layers of SiO₂, and a sensing medium. Only the Si and SiO₂ layers were randomly stacked, and the sensing medium was added after 5-unit cells. As a result, the structure is [(Si/SiO₂)₅/Ag/SL/Ag/(Si/SiO₂)₅]. Si, SiO₂ and Ag have refractive indices of 3.477, 1.44, and 0.0515 respectively. The refractive index of Normal Cells, Jurkat, HeLa, PC12, MDA-MB-231 and MCF-7 are 1.350, 1.390, 1.392, 1.395, 1.399, and 1.401 respectively. The thicknesses of the Si, SiO₂, Ag and sensing layers are 107.75 nm, 260.416nm, 4.5µm and 9µm, respectively. The intuitive approach is used to optimize the thickness and random designs. Using the aforesaid technique, the best structure is chosen from 1000 random constructions, and the structure is shown in figure. A transfer matrix approach determines the transmission and sensing properties of constructed random photonic crystals. For the normal incident of light, the simulation results reveal that the developed sensor has an excellent ability to identify cancer cells, with a sensitivity of 1627.45 nm/RIU. As it shows magnitude variations as well as wavelength shift for every distinct type of cancer cells, the results obtained can be very helpful in identifying the early stages of cancer cells with basic blood tests.

Keywords: Random Photonic crystal, Structural property relationship, Cancer cell sensor, Transfer matrix method, Silver.



Figure: Schematic and transmission spectra of Ag coated 1DRPC based biosensor

ICRTMD-2023/FIT/SIT/382 Assessing the Fracture Toughness and Dynamic Crack Propagation behavior of Epoxy Composites Reinforced with Chopped Carbon Fibers

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Abstract

This work mainly aims to investigate the fracture toughness and dynamic crack propagation behaviorof epoxy composites reinforced with chopped carbon fibers (CCFs). The CCFs were developed by recycling the waste carbon fiberfor developing a low-cost reinforcement for epoxy resins. The epoxy resins are brittle owing to their inherent crossed-linked structures and therefore, CCFs were used to improve the toughness of the epoxy composites. Different wt% of CCFs were added to the epoxy resin to improve its fracture toughness. The fracture toughness was evaluated following ASTM D5045 standard followed by high-speed imaging during the fracture. The addition of 1.5 wt% addition of CCFs into epoxy resin improves the K_{IC} value of the resulting epoxy composite by 72% compared to that of the neat epoxy sample. In addition to capturing the crack propagation during the SENB test, a high-speed imaging setup was used. The setup consisted of a high-speed camera (Phantom VEO 710) with a resolution of 1280 X 800 pixels and a maximum frame rate of 7400 fps.

Keywords: Epoxy Composite; Chopped Carbon fiber; Fracture toughness.



ICRTMD-2023/FIT/SIT/383 Nonlinear absorption coefficient and refractive index of scattered Stokes mode in n-type doped gallium arsenide

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Abstract

Many scientists have become interested in the experimental and theoretical studies concerning the measurement of nonlinear optical susceptibilities in various media due to their potential applications in the development of more modern coherent laser sources over a wide frequency range, including parametric amplifiers and oscillators, optical switches, phase conjugate mirrors, and above all, parametric amplifiers and oscillators. Semiconductors have been the obvious choice as host media for the study of nonlinear optical phenomena, as opposed to materials like gases and liquids, because of the accessibility of sophisticated fabrication technology and the experimental observations of giant optical nonlinearities in the band-gap resonant transitions. Gallium arsenide (n-GaAs), which has a many-valley band structure, has an advantage over other semiconductor materials in the field of device construction due to its NDR feature. I calculated the nonlinear propagation of a high frequency pump radiation in an n-GaAs sample in the region of negative differential resistivity using a hydrodynamic model of plasma in this research. In order to help the pump wave move electrons from the lower conduction valley to the upper satellite valleys in n-GaAs and therefore increase the effective mass of electrons, a d.c. electric bias is introduced. The effective mass's energy dependence and the sample's piezoelectric properties lead to the nonlinearity. It is discovered that the induction of fourth-order nonlinearity in the sample is caused by the energy dependence of the mass in the region of negative differential resistivity. It is discovered that the nonlinear optical properties of the sample are significantly influenced by the negative differential resistivity area in n n-GaAs.

Keywords: Nonlunear refractive index; nonlinear absorption coefficient; gallium arsenide.

Faculty / Scientist Talks

ICRTMD-2023/FT/ST /119 Impact of Machining Environment on Surface Integrity of Co-Cr-Mo Biomaterial in CNC Precision Turning

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Abstract

The characteristics of the contact surface layer determine the practical uses of joint implants. Osteolysis caused by wear and debris and aseptic loosening are the reasons why metal-onmetal joint implants fail. Reducing the amount of debris released is essential to the prosthetic joint's long-term durability. Grain size gradients and ultrafine or even nanosized grains are produced in the surface region of various materials by severe plastic deformation (SPD) techniques, which have been exploited to modify the surface integrity properties. When compared to their predicted coarse-grained counterparts, these fine-grained materials frequently exhibit improved surface integrity qualities and improved functional performance (wear resistance, corrosion resistance, fatigue life, etc.). As a result, when CNC cutting a surface implant, precise machining parameters must be used to ensure surface quality. The current study focuses on how the wet and dry machining environment affect the Co-Cr-Mo biomaterials's machined surface integrity by using Taguchi DOE technique.

Keywords: Co-Cr-Mo Biomaterial, Surface roughness, Taguchi DOE, CNC Precision Turning & Dry and Wet Machining.

Design and Development of a Smartphone Spectrometer in Visible Domain

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Abstract

Optical spectroscopy is the scientific discipline addressing the interaction of matter with light through processes like emission and absorption. Various techniques, including emission spectroscopy, absorption spectroscopy, and fluorescence spectroscopy, contribute to this field. UV-VIS spectroscopy, a specific subset, operates on the principle that ultraviolet and visible light can excite π -bond and non-bonding electrons, causing absorption within the electromagnetic spectrum.

UV-VIS spectroscopy boasts diverse applications across various fields. The tool commonly employed for optical spectroscopy investigations is an optical spectrophotometer. In the current research, a spectrophotometer was innovatively developed, utilizing a smartphone's camera as the detection unit. This system integrates basic laboratory optical components—pinholes, lenses, prisms, gratings—with the smartphone's camera module, enabling visible spectroscopy within the 400-700 nm wavelength range. The design prioritizes simplicity and accessibility in optical components, taking into account the need for device miniaturization.

As a proof of concept, the smartphone spectrophotometer was demonstrated to measure absorption bands of commonly used color filters. Broadband light passing through these filters, positioned between the collimator and the cylindrical lens, allows transmitted light signals to be captured directly by the smartphone camera. This showcases the potential of using a smartphone as a spectrophotometer for practical applications. The resulting smartphone spectrophotometer is not only cost-effective but also robust and easily portable for field applications.

Keywords: Smartphone, Spectrometer, Camera, Color filters, Absorption bands

Preparation of CuZnS thin films by Chemical bath deposition method and its Characterizations

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Abstract

Among the different renewable energy resources, solar energy is significant because of its existence in the universe, low cost, and free high energy power. Constituent elements used for the fabrication of solar cells are nontoxic and abundantly available on Earth. In the present study, Copper Zinc Sulphide (CuZnS) samples were prepared on the glass substrate from the precursor solution (CuCl2, ZnCl2, TEA, NH3, Thiourea, and distilled water) at temperature 800C by chemical bath deposition method. The pH of the precursor solution was 11.61. Samples were prepared by varying the time of deposition and temperature. Structural, morphological and compositional characterizations of the sample were studied by using XRD, SEM and EDAX. The thickness of the sample was measured by using Profilometer.

Keywords: CuZnS; Chemical bath deposition; Preparation of thin film; Characterization.

Device simulation and optimization of HTL-free Perovskite solar cell with CH₃NH₃SnBr₃ as the absorber layer by SCAPS -1D software

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Abstract

Perovskite solar cells without a hole transport layer have gained popularity due to their stability and affordable manufacturing. In this work, device simulation of the solar cell structure is done using SCAPS-1D software with TiO_2 as the Electron Transport Layer while toxic-free compound CH3NH3SnBr3 as the absorber Material. The efficiency of the structure is found to be 12.63%. The cell performance parameters are further investigated by varying individual cell parameters such as absorber layer thickness and defect density, absorber layer doping concentration, ETL thickness, ETL doping concentration, temperature, series and shunt resistance while holding others constant. Simulation is repeated with optimised cell parameter values and it improves the efficiency to 23.93%.

Keywords: Simulation, Perovskite solar cells, HTL-free, Optimization.

Design and analysis of SiGe source based Gate All Around core shell dopingless nanotube Tunnel FET

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Abstract

In this article, Gate All Around tunnel field effect transistor with a core-shell dop-ing less nanotube is proposed with SiGe based Source (SiGe based GAA CS DL NT TFET). The major asset such as SiGe being the lowband gap material - in-creases the carrier charges movement inside the channel which in turn enhances the device characteristics and Doping-free charge plasma technology, which is li-able in designing it. The source and drain areas are produced using the appropri-ate metal working functions instead of doping, which is not employed in charge plasma processes. This Doping less technique effectively reduces the fluctuations caused by the random dopants. Attainment investigation of the SiGe based device structure is correlated with the Si based source device structure. Theanalog and RF analysis are made for both the devices to compare their electrical characteris-tics. The structure comparative analysis between Si based and SiGe based devices showcased that the proposed device's strong candidature for the fast switching and improved charge carrier concentrations. The proposed SiGe based GAA CS DL NT TFET device resulted in 2.95×10^{-5} (A/µm) and highest ratio of 5.68×10^{11} when compared to Si based source device. The enhancement of the devices with SiGe based source proves to yield better performance with respect to the na-noscale dimensions.

Keywords: SiGe source, Charge plasma Doping less, core shell gate, nanotube, Tunnel Field Effect Transistor.

UV-Visible Absorption Technique for Determination of Rate of Synthesis of Thiobarbituric Acids and their Knovenagel Derivatives

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Abstract

Several studies have been published on the synthesis and spectral properties of several thiobarbituric acids, azobarbituric acids. Thiobarbituric acids, azo dyes based on heterocyclic amines have been developed, and the resultant benzylidene derivatives of TBAs, dyes give higher tinctorial strength and brighter dyeing. The compounds containing amino-substituted thiocompounds compounds afford highly electronegative diazo components and consequently, provide a pronounced bathochromic effect compared to the corresponding benzenoid compounds. The introduction of substituent groups into the aromatic ring can completely change the nature of the electrode reaction because of their different sizes and orientations. The synthesized substituted barbituric and thiobarbituric acids generally showed good light stability, analyze their photophysical and spectroscopical properties. Barbituric and thiobarbituric acids has been employed as conjugating moiety due to its excellent charge transporting capability, polarizability, as well as tunable electrochemical and spectroscopic properties including enhanced molar extinction coefficients at longer absorption wavelengths. The various barbituric acids were chosen for the coupling components and are known to give highly stable and brightly colored dyes. The rates of optimization of reaction conditions during the synthesis of thiobarbituric acid and their Knovenagel derivatives measured the absorbance on UV-visible spectrophotometer.

Keywords: UV-Visible technique, Thiobarbituric acid, Thiobarbituric acid derivatives.

ICRTMD-2023/FT/ST /162 Green polysaccharide material for the removal of colour, TDS, COD and chloride from Dyeing effluent

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Abstract

Textile industries are responsible for one of the major environmental pollution problems in the world because they release undesirable dye effluents. The dyeing, finishing, and washing processes in the textile processing business require a lot of water, making it a water- intensive industry. The majority of dyeing enterprises either treat their effluents completely or only partially before releasing them into the environment. The ecosystem and human health may be at risk due to the discharge of these dye effluent and the structure of the persistent dye, which has hazardous qualities. According to animal research reports, dye ingestion has a wide range of negative effects, including carcinogenic, genotoxic, mutagenic and teratogenic effects. In addition, the non-biodegradable properties of organic dyes and the intensity of their colors have the power to decrease aquatic variety by obstructing sunlight from penetrating the water. Additionally, some of them have the potential to irritate the respiratory system, skin, eyes, and cause allergic dermatitis if eaten. Hence, the treatment of dye effluent is utmost essential before going to discharge in any ecosystem. In the present investigation, the synthetic dve effluent was collected from the textile dyeing unit and the physic- chemical characteristics were analyzed using APHA standard method. The results stressed to treat the effluent by using an eco-friendly green materials. The effluent was subjected to treatment with natural polysachharide dosages such as 0.1g, 0.2g, 0.3g, 0.4g, 0.5g of polysachharide isolated from Tamarindus indica L. Tamarindus indica L seed Polysaccharide was used for the removal of color, TDS, COD and Chloride from the black dye effluent. About 81% of TDS, 77% of COD and 76% of Chloride removal were obtained at 0.5g of dosage treatment of polysachharide proved the ability of coagulation and pollutant removal capability. The functional group changes in the natural coagulants and chemical sludge were analyzed before and after the treatment which were characterized by using the FTIR technique. The raw dye sample and treated dye sample were qualitatively analyzed by GCMS analytical method. Hence, the present study suggests that, the possibilities for the use of Tamarindus indica . L seed polysaccharides for the treatment of dye effluent.

Keywords: polysachharide, natural coagulant, Tamarindus indica L, dyeing effluent, TDS, COD.

Tuning Surface Plasmon Resonance of Gold using Rippled Si Surface

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Abstract

Gold nanoparticles (NPs) have attracted much attention from researchers since ancient times and have been an area of enormous and exponentially growing interest because of their applications in solar cells, nonlinear optical devices, sensors, etc. They show fascinating surface plasmon resonance (SPR) property which depends on the size and shape of NPs, and the environment including separation between the nanoparticles. In this work, we report the SPR properties of Au nanopillars developed on rippled Si substrates. The templated Si surface was prepared by the bombardment of Ar ions at 60° with respect to the Si surface and ripple structures were developed with varying ion fluence. to fabricate ripples on the surface. A 5 nm thin layer of Au was then deposited on the rippled surface and the surface plasmon resonance (SPR) was studied using UV-visible spectroscopy. Further, atomic force microscopy (AFM), was used to get the surface morphology of the prepared samples. The AFM confirmed that the deposited gold is in nanopillar form and the growth, shape, and size of gold nanopillars is governed by rippled surface. A large aspect ratio has been observed for the nanopillars, resulting in the red-shifted and split SPR band.

Keywords: SPR, Au Nanoparticles, Anisotropic growth, Nanopillars.

Electrical Charge Transport Exploration 1 of CSA-doped poly (o- methylaniline); A Conducting Polymer

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Abstract

The polymerization of the poly(o-methylaniline) (PoMAni) doped with the camphor sulphonic acid (CSA) was carried out by chemical method using ammonium peroxi disulphate (APS) as an oxidizing agent. The polymerizations were carried out by the optimization process and are based on the dopant to monomer ratio. The synthesized polymers were characterized by using XRD, UV-vis and FTIR spectroscopy. The doped and dedoped samples confirmed the polymerization of poly(o-methylaniline). The presence of the band at 819.59 cm⁻¹ in FTIR spectra belongs to the characteristics para-substituted aromatic rings in PoMAni-CSA confirmed the successful polymerization. The temperature dependence electrical conductivity of PoMAni samples were examined in the wide temperature range 300K - 430 K. The electrical conductivity 1.0×10^{-7} Scm⁻¹ among all optimizes samples was found to be maximum at molar ratio 3. The electrical charge transport mechanisms were examined with help of different charge transport models; Mott-variable range hopping (M-VRH), Arrhenius and Kivelson model. The charge transport mechanism based on the different parameters revealed that Kivelson model shown there applicability in the temperature range 350-430 K, however Mott (1-2-3 D) shown there existence in the temperature range; 300-370 K, 300-380 K, and 300-420 K respectively. Kivelson model existed in 300-360 K range. The Arrhenius model was found to explain charge transport in higher temperature range, while Kivelson model explained the transport in lower temperature range. However, Mott three-dimensional VRH model was observed to be operative in the longest temperature range. Therefore, a mixed charge transport mechanism is suggested for poly(o-methylaniline).

Keywords: Poly(o-methylaniline), CSA, M-VRH model, Kivelson model, Arrhenius model.

ICRTMD-2023/FT/ST /210 Growth and properties of metallic and insulating molybdenum oxide thin films

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Abstract

We have studied the effect of Fe doping on the structural, electrical, and magnetic properties pulsed laser deposited of MoO_x thin films on Si substrate. Detailed analyses of the structural properties suggest that the grown phase of molybdenum oxides and its orientation strongly depend on the Fe doping and Oxygen oxygen partial pressure. The resistivity behaviour of the films prepared in vacuum condition shows intriguing behaviour. It is observed that the film reveals anomalous behaviour at 280 K. The films grown at 10 mTorr OPP also reveal strikingly different nature with and without doping . While the film shows metallic behaviour in the entire temperature regime 300K-4K, These observations clearly reveal that Fe extremely govern the structural and electrical properties of the molybdenum oxide films.

Keywords: Thin film, structural property, Magnetic properties.

Enhancing Durability and Water Repellency of Cement Blocks through Nanostructured SiO₂ Coating

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Abstract

Our comprehensive analysis reveals that the integration of nanostructured SiO_2 particles (approximately 125 nm - syntehisized using green approch) into the cement surface effectively impedes the development of microcracks. Additionally, the inclusion of nanostructured SiO_2 brings about a significant transformation of the cement block's surface, resulting in a superhydrophobic state with a water contact angle surpassing 152°. This superhydrophobicity not only shields the surface from moisture-induced damage but also imparts self-cleaning properties, making it an appealing choice for a variety of construction applications. The implications of these findings for the construction industry are noteworthy, offering a novel and efficient approach to extend the lifespan of cement-based structures while minimizing maintenance requirements. The incorporation of nanostructured SiO_2 opens avenues for sustainable and cost-effective construction practices, ensuring the resilience of infrastructure across diverse environmental conditions.

Keywords: Nanostructured SiO₂, Microcrack mitigation ,Superhydrophobicity,Water contact angle.

Effect of Reinforced Particulates on mechanical properties of AA5059 Based Metal Matrix Composite

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Abstract

The aluminum-based composites are demanded in the aerospace, marine and automobile industries, due to their good mechanical properties and high strength to weight ratio. The present work aimed to develop the AA5059 based composite with SiC, B_4C and Al_2O_3 as a reinforcement. The composites are prepared using the stir casting technique, in which reinforcements are mixed to the AA5059 matrix in different compositions. The Composites are subjected to microscopic analysis to know the porosity and distribution of the reinforced particles in the composites. Hardness and tensile test were performed on the prepared samples to find the mechanical properties of the composites. The composites microstructure shows that SiC, Al_2O_3 , B_4C powders are distributed uniformly in throughout the composite. The maximum tensile strength of composites is obtained as 180 MPa at cast condition of Al5059+6%SiC+6%Al2O3+6%B4C.

Keywords: AA5059; Stir Casting; Microstructure; Mechanical Properties.

Magnetism in semiconductor nanomaterials (A comparative study)

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Abstract

Nanotechnology has brought about tremendous impact on the semiconductor industry. It has resulted in increased efficiency, sensitivity and manufacturing of a device in cost-effective manner. This advanced technology has replaced almost whole of the conventional semiconductor industry like photonic devices, photovoltaics, transparent electrodes, high electron mobility transistors, sensors, short term memory in a computer, energy harvesting and energy storage devices. Semiconductor nanomaterials have structural, morphological, optical, electronic and magnetic properties, which are significantly different from those of their bulk materials. Semiconductor nanoparticles (NPs) also called quantum particles or quantum dots which form a unique category of new material for which size dependent properties are realised. This article focuses on the introduction to these semiconductor NPs and comparative study of induced magnetism by adding dopants in wide band semiconductors as ZnO and ZnS, so that they can be employed for further research in the diverse area of nanotechnology. Semiconductor nanomaterials can be used by almost whole of the scientific community in the fields like physics, chemistry, biology, computer science and engineering.

Keywords: Wide band gap (WBG) semiconductors, semiconductor nanoparticles (NPs), magnetism.

ICRTMD-2023/FT/ST /257 Experimental Analysis of Metal Matrix Composite on AL6061/SiC/B4C/Fly-Ash

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Abstract

Composite materials of Aluminum alloys Al6061 have high strength to weight ratio. High-strength forging alloy Al6061 that can be heat treated. Similar to the Al7075 alloy, but with better toughness and tensile strength, it has a superb balance of toughness and strength. The engineers have studied this metals characteristic. The problems associated with employing aluminum alloys in manufacturing have been resolved by contemporary manufacturing techniques. This led to a great desire for the application of aluminum alloy in all engineering domains. Due to their vital qualities including enhanced specific strength, high temperature and wear resistance, aluminum metal matrix composites are becoming increasingly popular for automotive, aerospace, agricultural farm machinery, defense sector, and many other industrial applications. By adding reinforcements made of Boron Carbide (B4C), Silicon Carbide (SiC), and Fly-Ash to the Al6061 matrix, the mechanical parameters such as tensile strength, compression strength, and hardness can be improved. Creating four different with varying makeup and performing Tensile test, Hardness test, Bending test and Micro-structure on each specimen.

Keywords: Aluminum 6061, Boron Carbide, Silicon Carbide, Fly-Ash, MMC(Metal Matrix Composite), Tensile test, Hardness test, Bending test, Micro-Structure.

Nanocellulose Supported Copper Ferrite Nanoparticles: Synthesis from Simarouba glouca Leaf Extracts and Application

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Abstract

Ferrites are ferromagnetic oxides having wide variety of applications such as magnetic resonance imaging, electronic devices, information storage[1] and drug delivery[2] due to their magnetic properties, adsorption of toxic substances and gases [3-9], chemical sensors [10-11 and pigments [12]. Different industrial processes like oxidative dehydrogenation of hydrocarbons, decomposition of alcohols and hydrogenperoxide, treatment of exhaust gases, oxidation of compounds such as CO,H2,CH4 and chlorobenzene[13]. Nanocellulose prepared from agricultural waste enhances the performance of copper ferrite nanoparticles. The high catalytic activity of nanocellulose supported copper ferrite nanoparticles is due to large surface area and the abundant of hydroxyl groups induced immobilization of copper ferrite nanoparticles make the nanohybrids stable. In the present work, we reported a novel method of synthesizing $CuFe_2O_4$ nanoparticles using aqueous leaf extract of Simarouba glouca plant. Nanocellulose is obtained from leaf sheath of banana pseudostem by physio- chemical method. Nanocellulose - copper ferrite nanohybrid is prepared by ex-situ method. The prepared nanomaterials are characterized by XRD, FT-IR, UV, SEM, TEM, Photoluminescence and XPS method. The photocatalytic activity of the materials are performed using malachite green and congo red dye with visible light irradiation. These study reveals that photocatalytic ability of the material enhanced to nearly 100 percentage with nanocellulose CuFe₂O₄ nanohybrid due to large surface area of nanocomposite compared to other materials. The present investigation reveals that prepared nanocomposite is future adsorbent material for water purification.

Keywords: Copper ferrite, Simarouba glauca, malachite green, Congo red, Photocatalysis.

Synthesis and Photoluminescence Properties of Trivalent Rare Earth Doped MgY₂Al₄SiO₁₂ Phosphor

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Abstract

This work involves a series of trivalent europium doped MgY2Al4SiO12 garnet phosphors were synthesized by wet chemical method as sol-gel synthesis. The phase purity and crystalline nature of MgY₂Al₄SiO₁₂:xEu³⁺ phosphors were confirmed by X-ray diffraction (XRD) analysis and matched with JCPDS file. Under the excitation of 394 nm, MgY₂Al₄SiO₁₂:Eu³⁺ samples showed an intense emission peak at 592 nm and 612 nm in the orange-red region. Photoluminescence (PL) emission intensity increased up to 5 mol %. This synthesized phosphor can be used as orange-red light emitting phosphor in LED applications.

Keywords: Phosphor, Sol-gel method, Photoluminescence, XRD.

ICRTMD-2023/FT/ST/312 Experimental and computational investigation of Imino-5-methylsulpanyl-1,7-dihydro-[1,2,4] triazolo[1,5-a] pyrimidine-6-carbonitrile

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Abstract

The current reviews agreements with a detailed examination on the computational study of Imino-5methylsulpanyl-1,7-dihydro-[1,2,4] triazolo[1,5-a] pyrimidine-6-carbonitrile by using density functional theory (DFT). The optimized molecular geometry, bond lengths, bond angles, atomic charges of the titled compound has been investigated by Density Functional Theory (DFT) using standard B3LYP method with 3-21+G basis set using Gaussian 16 W package. The HOMO to LUMO transition implies an electron density transfer.

Keywords: DFT, Imino triazolo, HOMO- LUMO study.

ICRTMD-2023/FT/ST /316 Development of Size and Shape dependent model for vibrational frequency of nanaocrystals

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Abstract

The properties of bulk materials depends on their structure. But at nanoscale size and shape of the materials are the important factor. High surface to volume ratio is the most important property of materials. Thermodynamic properties of the materials has been affected by this high surface to volume ratio. Qi and Wang has given the expression for cohesive energy. The expression given by Qi and Wang has been extended to study the energy gap, vibrational frequency and static dielectric constant for nanoparticles, nanowires and nanofilms. Energy band gap increases with increase in size of nanocrystals while vibrational frequency decreases with increase in the size of nanocrystals. Dielectric constant is also decreases with increase in the size. Bulk and nanomaterials have different properties. The valid theoretical model about the size effect about the size effect of elastic modulus and vibrational frequency is significant to guide the application of nanomaterials. Vibrational spectra of metal nanoparticles are the signature of their structure and vibrational spectra of metal nanoparticles has been used to determine the low temperature behavior of the thermal properties. Vibration is actually a mechanical phenomena. Mechanical system vibrates at one or more of its natural frequency. Vibrational frequency has been used many years to identify bonding arrangement of molecules. Each bond has its own frequency so vibrational frequency yields the information on molecular structure. In the present paper, we will develop a simple theoretical model to understand the variation of vibrational frequency of nanomaterials with size. We also include the shape factor in present study. We will study size and shape dependence of vibrational frequency for different nanomaterials. We will also compare our theoretical results with suitable experimental data. Our theoretical results will be in good agreement with the available experimental data which supports the validity of model proposed.

Keywords: Vibrational frequency, Size, Shape, Surface to volume ratio and Cohesive energy.

Role of artificial intelligence (AI) and machine learning (ML) in the corrosion monitoring processes

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Abstract

When it comes to the upkeep of engineering structures in a variety of industries, corrosion monitoring systems are an extremely important component. In particular, applications such as storage tanks for hazardous chemicals and weight-bearing structures of large engineering constructions are at the forefront of providing attention to relevance. This is due to the fact that failures experienced by these applications can potentially result in catastrophic consequences. As a result, contemporary methods make use of the application of concepts connected with machine learning and artificial intelligence in order to efficiently monitor corrosion. As a consequence of this, the monitoring system is able to provide the control system of the industry with minute-by-minute updates regarding the condition of an engineering. Therefore, the catastrophe is prevented to a significant degree, and there is a significant possibility of lowering the costs associated with technical procedures that require maintenance. Within the scope of this paper, a comprehensive analysis is conducted on the applications of artificial intelligence and machine learning techniques that are utilized in corrosion monitoring systems across a wide range of industries. Through this assessment, the solutions and efficient corrosion monitoring methods that are specific to the domain are made available. Consequently, the purpose of this work is to determine the appropriate technique of monitoring systems for each and every corrosion-related disorder.

Keywords: Artificial Intelligence, Machine learning, Corrosion monitoring system, Oil and gas industries.
Student Talks

ICRTMD-2023/ST/105

Novel Modification of Activated Charcoal Sheet with Polypyrrole and Silver Nanoparticles for Removal of Hexavalent Chromium in Water Treatment Processes

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Abstract

In the present study, we developed novel activated charcoal (AC) sheet, silver nanoparticles (AgNPs), and polypyrrole (PPY) conducting polymer nanocmposites, referred to as PPY-AgNPs@AC CPN. The CPN materials were investigated for efficient adsorptive removal of hexavalent Chromium (Cr+6) ions from water in batch mode water treatment processes. We characterized the synthesized CPN materials using HR-FESEM (high-resolution field emission scanning electron microscopy), XRD (X-ray diffraction), FTIR (Fourier-transform infrared spectroscopy), and EDS (energy-dispersive X-ray spectroscopy). The PPY-AgNPs@AC CPN showed an excellent Cr+6 ions adsorption efficiency (Ad%) of 99.8%, along with a high adsorption capacity (qe) of 380 mg/g. Furthermore, the various parameters affecting adsorption, such as pH, adsorbent dose, initial Cr^{+6} ions concentration, temperature, and contact time were extensively studied. The study evaluated PPY-AgNPs@AC CPN as not only highly efficient Cr+6 ions adsorbents but also cost-effective and eco-friendly alternatives. The PPY-AgNPs@AC CPN exhibited enhanced recycling performance over five cycles.

Keywords: Heavy metal ions; conducting polymer nanocomposites; activated charcoal; silver nanoparticles; polypyrrole; hexavalent chromium.

MXene- Polymer Nanocomposites for Energy Applications

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Abstract

Development of sustainable energy materials is considered as one of the promising fields of research as the demand of renewable energy resources is increasing day by day. MXenes are considered as potential candidates used to fabricate energy storage, harvesting and energy conversion devices. MXenes are transition metal carbides, nitrides and carbonitrides. These two dimensional materials are generally represented by the formula MnXn+1 where M is any early transition metal and X is carbon or nitrogen. The unique characteristics of MXenes include high conductivities comparable to metals and high negative zeta potential, high surface area with hydrophilic properties and exceptionally good mechanical properties. The applications of MXenes for the development of electrode materials can be enhanced by incorporating them into a polymer matrix. Reinforcement of a polymer matrix using MXenes can effectively improve the dielectric properties of the materials and possesses high specific capacitance and energy density. MXene-polymer nanocomposites exhibit tremendous mechanical, thermal, and electrical properties and it found applications in various energy storage devices like batteries, supercapacitors and utilized in EMI shielding and hydrogen/oxygen evolution reactions. Development of flexible electronic devices with superior properties can be made possible by utilizing highly efficient MXene-polymer nanocomposites.

Keywords: MXenes; Polymer nanocomposites; Electrode; Dielectric properties; Super capacitors; EMI shielding.

Co-existing Dual Morphology of Single-Phase Molybdenum Trioxide: Unlocking Enhanced Electron Transfer Characteristics

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Abstract

The dual morphology of single-phase molybdenum trioxide (MoO3) has emerged as a promising avenue for unlocking enhanced electron transfer characteristics for solar cell applications. In the present work, MoO₃ was synthesized by one-step hydrothermal synthesis route which resulted in a unique combination of nanorods and nanospheres in a single material. This controlled morphological heterogeneity enables the exploitation of diverse surface structures, resulting in improved electron transfer properties. The presence of nanorods and nanospheres in the same MoO₃ sample offers tunability and versatility in tailoring the material's properties. The nanorods provide an elongated structure, presenting a higher surface-to-volume ratio. This aspect enhances the material's efficient charge transfer characteristics. On the other hand, the nanospheres contribute to the overall stability of the material and promote enhanced electron transport due to their spherical geometry. The coexistence of these two morphologies facilitates the creation of interfacial regions within the single-phase MoO₃ material. These interfaces serve as sites for synergistic electron transfer between the nanorods and nanospheres, promoting efficient charge transport pathways and minimizing charge recombination. Cyclic voltammetry show a unique behaviour representing only electron transfer property without any anodic peak. Nyquist plot reveals Warburg diffusion showing the excess of electron production, which is suitable for solar cell application.

Keywords: Dual Morphology; Electrochemical analysis; Cyclic Voltammetry; Nyquist Plot.

ICRTMD-2023/ST/112 Room-Temperature Ethanol Sensor based on novel ZnFe₂O₄ gel

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Abstract

The objective of creating low temperature gas sensors has stimulated research into creating new incredible materials with large surface for quick response. In this investigation, for the low temperature ethanol sensing, we created a unique zinc ferrite based gel, using a hydrothermal approach. The morphological and structural investigation of synthesized gel was done using XRD, FESEM along with EDS and UV spectroscopy. The sensing experiments findings indicate a good response (Ro/Rg = 19) at 25°C temperature in the presence of 50 ppm ethanol with a very low limit of detection. GCMS was used to confirm the room temperature conversion of ethanol into acetaldehyde through oxidation. Additionally, the developed sensor has an incredibly quick response time of 27 seconds and recovery time of 11 seconds. The sensor not only gives better response and recovery, but also provides long term stability with time. This research may open up novel avenues for developing low-temperature ethanol sensors for reliable and efficient monitoring of the rising concern regarding the indoor atmosphere.



Fig.1. Sensing response of ZnFe₂O₄ based sensor at different ethanol concentrations.

Keywords: Zinc Ferrite, ethanol sensor, sensitivity, LOD.

Exploring the Potential of Tin-Doped Barium Hydride for Advanced Optoelectronic and Catalytic Applications

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Abstract

In this study, we report the synthesis of tin-doped barium hydride using the coprecipitation method. The structural analysis conducted through X-ray diffraction (XRD) confirmed the orthorhombic crystalline structure of the synthesized material. The optical properties were investigated via UV-vis spectroscopy, revealing a band gap of 4.07 eV and a prominent absorbance peak at 230 nm. Additionally, field emission scanning electron microscopy (FE-SEM) images displayed polyhedral-shaped particles of nanoscale dimensions, providing valuable insights into the morphological features of the material. The observed band gap and absorbance characteristics suggest the potential of the synthesized tin-doped barium hydride for various applications. The wide band gap makes it a promising candidate for optoelectronic devices, while the small particle size, as revealed by FE-SEM, could contribute to enhanced catalytic and sensing properties. Furthermore, the unique structural and optical properties may find applications in photocatalysis, photovoltaics, and sensor technologies. This research not only contributes to the understanding of the synthesis and characterization of tin-doped barium hydride but also opens avenues for exploring its diverse applications in advanced materials science.

Keywords: Barium Hydride; Tin; Optical Analysis; Morphological Analysis.

Sintering and Its Role in Modifying Magnesium-Zinc Spinel Ferrite: An Analysis of Structural, Morphological, and Magnetic Traits

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Abstract

This detailed investigation presents the intricate fabrication and exhaustive analysis of $Zn_{0.2}$ Mg_{0.8}Fe₂O₄ spinel ferrite nanoparticles, synthesized using the advanced sol-gel auto combustion method. Central to this research is the in-depth exploration of the nanoparticles' structural, morphological, and magnetic aspects, aiming to provide an extensive comprehension of their attributes and potential practical uses. From a structural standpoint, the study employs sophisticated X-ray diffraction (XRD) methodologies to ascertain the development of a uniform, single-phase spinel structure. XRD's precision is pivotal in accurately determining the crystallite sizes, which in this instance span from 21.01 to 42.77 nanometres. Such a range in size is essential for assessing the nanoparticles' applicability across diverse technological sectors. The research further utilizes Fourier transform infrared spectroscopy (FTIR) to examine the vibrational attributes of the nanoparticles. The FTIR findings display pronounced vibrational bands at 570.20 cm⁻¹ and 410.13 cm⁻¹, indicative of tetrahedral and octahedral coordination sites in the spinel structure, respectively. These results are key in understanding the ferrite nanoparticles' intricate internal composition. Morphological examination is conducted through field emission scanning electron microscopy (FESEM), offering insight into the particles' granular composition, and highlighting a varied grain size distribution. This diversity is crucial for gauging the nanoparticles' surface characteristics and reactivity in different settings. Magnetic properties are thoroughly evaluated using vibrating sample magnetometry (VSM). This analysis is essential for verifying the nanoparticles' ferromagnetic nature. The samples all exhibit multi-domain structures, evidenced by Mr/Ms ratios ranging from 0.148 to 0.177, reflecting the magnetic strength and orientation within the nanoparticles. This aspect is vital for their use in magnetic storage, sensing technologies, and biomedical applications.

Keywords: Spinel Ferrite; Nanomaterials; Structural; Morphological; Magnetic.

Optimizing Solar Panel Efficiency Through Active Cooling Techniques: A Comprehensive Research Exploration

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Abstract

Energy is the prime force for the development of the human being. This energy demand is continuously increasing with the development and population rise. International energy outlook expected that the energy demand will be increased by 37% till 2030. Currently, most of the energy demand is fulfilled by the non-renewable energy sources. The energy supply from the non-renewable energy source raise concern about the availability and the environmental quality. So, renewable energy source like geothermal, hydro energy, biomass, solar energy, etc can alter this problem. Solar energy is most promising renewable energy source due to its availability at most of the geographical location and long-life span. Photovoltaic (PV) cell is the most promising device to captured solar energy. But the problem associated with PV like poor thermal management and efficiency are the key barriers against its popularity. In recent time researcher have developed various medication like water cooling system, thermal energy storage system, nanoparticle integration in PV system to maintain the cell temperature and efficiency enhancement. It was found the overall efficiency was improved in between 2-7%. It was also observed that the integration of thesemedication increases the cost and reduce the life of the PV. It canneed to be optimize to reduce the cost and improve the life.

Hydrothermally Synthesized Nickel-Doped FeS₂/WS₂ nanocomposite as Supercapacitor Electrode Materials

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Abstract

Recently, Transition-metal sulfide materials, have attracted tremendous attention as active electrode materials for supercapcitor applications. Of these, Tungestun disulfide (WS₂) is an emerging electrode candidate for supercapcitor devices owing to their intrinsically layerd structure, large surface area, and larger interlayer spacing (6.18 A^{o}). Despite these advantages, mostly WS₂ based noanomaterials do not exhibt sufficiently electrical properties unmatched with predominantly used non-zero gap highly conductive grapheme, which hindsers the direct applications of stand-alone WS2 based materials for supercapcitors. To our best knowledge, nickel-doped FeS₂/WS₂ nanocomposite will first time reported as an active electrode for high-performance supercapacitor applications. In the present work, nickel-doped FeS2/WS2 composite were prepared through cost-effective, environment friendly, and efficient, one-step solvothermal process. The surface morphplogy of the as-synthesized Ni-doped FeS₂/WS₂ nanostructures were characterized by scanning electron microscopy (SEM) which indicates that the prepared sample consists of WS₂ Neolamaeckia cadamba/flower-like hetrostructure. This is of first type reported structure as active electrode for supercapacitors. Size and other surface properties of morphologies were essamined by transmission electron microscopy (TEM). The crystal structure and phase analysis of the as-synthesized Ni-doped FeS₂/WS₂ nanostructures, was examined by X-ray diffraction (XRD). The elemental composition of the as-synthesized sample was examined by EDX and XPS analysis. As an electrode, nickel-dopedFeS2/WS2 neolamarckia cadamba/burflower-like hetrostructure exhibited a high capacity of 2565 mFcm⁻² at a current density of 0.35 mA cm⁻² and retained a high specific capacitance of nearly 94% after 5000 cycles. Besides this, the WS2-based supercapacitors, particularly, show and exceptional charge-discharge performnance. Moreover, nickel-doped FeS2/WS2 neolamarckia cadamba/burflower-like hetrostructure exhibited better capacitive property as compare to WS₂, and FeS₂/WS₂ electrodes. The low cost and their excellent electrochemical performances suggest that nickel-doped FeS2/WS2 neolamarckia cadamba/burflower-like hetrostructure electrode materials have huge potential in promising applications not only on high-performance supercapacitors but also on other advanced energy-storage devices.

Keywords: Nickel-Doped FeS₂/WS₂; Flower-like hetrostructure; Hydrothermal method; Supercapacitor; specific capacitance.



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161

ICRTMD-2023/ST/132

Carboxymethyl cellulose/β-Cyclodextrin/nickel cobaltite-based nanocomposite for the removal of malachite green

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Abstract

Wastewater contamination have been one of the great concerns for many decades. Dyes are colorant material which can interfere with the life of the aquatic organisms and decrease the quality of the water. Adsorption is one of the simple and cost effective approaches to remove the dye contamination from the wastewater. Use of biodegradable materials as an adsorbent to remove wastewater contamination is more favoured due to its environment friendly nature. In the present work, a novel nanocmposite based on biodegradable carboxymethyl cellulose, β -cyclodextrin, and succinic acid reinforced with nickel cobaltite (NiCo₂O₄) was used as an adsorbent to remove malachite green (MG) contamination. The adsorption efficiency of the synthesized composite was studied under different conditions. Artificial neural networking (ANN) was trained to forecast the removal of malachite green using composite material. Isotherm, thermodynamics, kinetics investigations were also carried out to determine the effectiveness of the uptake of MG by the composite. The results revealed that the novel composite material can be used to remove MG from the aqueous stream.

Keywords: Carboxymethyl cellulose; Biopolymer; Artificial neural networking; Cobaltite; Adsorption.

Salt's function in creating brick-shaped nanoparticles based on carrageenan

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Abstract

In the pharmaceutical industry, the use of polymers whether in their natural form or through chemical modificationis crucial. Grafting polymers for drug delivery and research purposes has drawn attention for decades. Because of their intriguing qualities, polymer-based nano-formulations are very well-liked. Controlling dimensions at the nanoscale, however, is a very difficult task. The goal of the current study is to create brickshaped nanoparticles by observing how the shape of the particles changes when salt is added. The desolvation method developed the formulation in a straightforward, eco-friendly manner. In the initial experiment, which was intended to obtain a gelling-free solvent, it was discovered that adding salt (NaCl) to water helped to felicitate the solution form without any gelling properties. With this in mind, an aqueous solvent was used while stirring continuously. Dropwise addition of more ethanol demonstrates turbidity, which validates the formation of nanoparticles. The particles began to settle after up to three hours of stirring. They took the shape of white bulk filters, which were used to gather the dried carrageenan nanoparticles and analyses them using TEM and SEM. As a cube-shaped nano has a larger volume to surface area than other shapes, shape plays a significant role at the targeting site. It's possible that the presence of chloride ions (NaCl) with controlled corner truncation is what produced this brick-like shape. Among their many advantages over other nanoparticles, brick-shaped nanoparticles also affect cellular uptake, site specificity, and target delivery. The other benefits associated with shapes include their interaction with cell membranes, blood vessel flow, and the ability of macrophages to clear reticuloendothelial organs based on their shape. Additionally, it is a controlled release formulation that can be used for antitumor, target drug delivery, and antiviral treatments.

Keywords: Polymer, nanoparticle, desolvation, Chloride ion, brick shape, salt.

Fracture Properties and computational characterization of cracks in Internal combustion engine crank shaft

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Abstract

The crankshaft holds a very important role in internal combustion engines by converting the reciprocating motion of pistons into rotary movement in the shaft and helps keeping the combustion in time. In this paper, detailed analysis with a crack in the crankshaft using fracture tool in static structural analysis in Ansys, to understand its stress state. For this objective a crankshaft of a motorbike was designed using normalized low alloy steel as material. Cracks were introduced in different orientations around the lubrication hole (crank pin) to see the effects of tensile forces on these different orientations, simulating a working condition of a crankshaft inside an engine. When the length of crack is perpendicular to the force applied, the value of stress intensity factor (k_1) obtained was very high. Values of K1 were found to be initially increasing from 40.608 MPa mm^{0.5} to 103.53 MPa mm^{0.5} and then decreasing to a value of 37.187 MPa mm^{0.5}. When the length of crack is parallel to the applied force, the value of stress intensity factor (k_1) obtained was very low and depending on the orientation of crack the value of the stress intensity factor would become negative in value. Smart crack growth tool was utilized to study the propagation of the crack. The results obtained were then compared to W.D Pilkey's Analytic method for calculation of stress intensity factor and was found to be 43.404487 MPa mm^{0.5}.

Keywords: Crankshaft, Crack, Stress Intensity Factor, Smart Crack Growth, Fracture Tool, W.D Pilkey Analysis of Crack.

Creep materials characterisation under high stress and high temperature conditions of AI6061 alloy

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Abstract

This study presents a comprehensive analysis of the creep behaviour of a standard rectangular specimen of Aluminum Alloy (6061-T6) through finite element simulations using ANSYS software. The primary focus is on investigating the specimen's response to varying stress loads and elevated temperatures. Boundary conditions were applied to the specimen, with a stress load exerted on one face. The time-dependent strain responses were analyzed, revealing a compelling correlation between applied stress, temperature and the specimen's rupture time. The findings indicate that higher stress levels and elevated temperaures contribute to a significant reduction in the material's time to rupture. It was at the creep (strain rate) goes on increases or decreases by gradually increasing the temperature to maximum limit. Increasing the load or temperature, has increase the strain rate and specimens got fractured before the natural time.

Keywords: Finite Element Analysis, Creep Strain, Temperature, strain rate

Light Material Selection and Dynamic Analysis of Differential Gerabox for four wheeler automobile

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Abstract

Differential Mechanism plays a vital role in enhancing the stability of an automobile as it contains the set of gears and shafts that facilitate the division of torque between the drive wheels, which help in the smooth turning of the Automobile. The Differential gearbox is subjected to different loads and torque as a result of this, there is deformation and various stress and strain developed while designing differential gear it is important to analyze stresses for safety operation. In this project, we made the model in Solidworks and then imported it to Ansys workbench for static and dynamic analysis, because static analysis focuses on evaluating the gearbox's ability to withstand static load ensuring that it operates in a safety margin and does not experience excessive deformation or stress concentration. Dynamic analysis is a critical component of this study which aims to investigate the gearbox behavior under varying loads and operating conditions to determine deformation, elastic strain, etc with different materials such as Aluminium, Cast Iron, Magnesium Alloy, Structural Steel, and Titanium Alloy. This analysis provides valuable insights into the gearbox performance and helps to identify potential areas for design optimization and strengthening. This result helps us to choose the best suitable material among them for Differential gear. This study contributes to enhancing the durability and reliability of differential gearbox.

Keywords: Differntial Gearbox, Static Structural, Explicit Dynamics, Total Deformation, Stability, Simulation.

Computational Stability Analysis of Francis Turbine Impeller Using Finite Element Method

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Abstract

This project uses ANSYS to analyze a Francis turbine rotor, aiming to understand its behavior better. This research project covers critical aspects such as critical speeds, deformations, deflections, stability conditions, modes, and natural frequencies of rotor under various rotational speeds of rotor. the impeller, a crucial part of Francis turbines, is examined in this research. We simulate real-world scenarios by applying rotational velocities as the main input. To mimic practical turbine conditions, we set up boundary conditions with bearings placed at the shaft ends to analyse different situations with stiffness and damping values and added remote displacement at the ends of the shaft to restrict deflection only in axial direction.

The modal analysis shows how the impeller responds to loads. Identifying critical speeds by Campbell diagram helps us understand potential peak resonance zones, Stability criteria, drawn from the analysis, contribute to a complete understanding of how the impeller reacts to dynamic forces also indicates the conditions when the rotor system gets unstable due to higher frequency, Deformation and deflection analyses how the impeller's structure behaves under different loads, ensuring its reliability in real-world applications, Modes and natural frequency analyses explore the vibrational characteristics, guiding us in refining the impeller's design to reduce operational risks.

In conclusion, this project is a significant step in turbine rotor analysis, combining theoretical insights with realworld input conditions. The knowledge gained from the modal analysis plays a crucial role in improving turbine design, ensuring the sustainable and efficient use of resources. This study adds to our understanding of rotor structural behaviour and turbine dynamics making strides towards achieving optimal turbine performance.

Keywords: Modal analysis, Ansys, Impeller, Stability, Deformation.

ICRTMD-2023/ST/142 Enhancement of Structural strength and stability Analysis of Trellis Bike Chasis using Finite element method

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Abstract

In the ever-progressing landscape of machine design, this study at hand addresses the critical aspect of bike chassis design. Employing cutting-edge technologies, this study uses Ansys R1 2023 to optimize the performance and reliability of a bike chassis. A Trellis Chasis is chosen for the study. The initial phase involves the creation of a detailed bike chassis model using SOLIDWORKS, laying the foundation for subsequent analyses. Ansys, a robust FEA tool, is then employed to subject the CAD model to modal and structural analyses. The goal is to identify potential weaknesses, resonant frequencies, and stress concentrations within the chassis structure. The obtained results from this initial analysis serve as a baseline for the subsequent design modifications. Based upon the insights garnered from the analysis, the CAD model undergoes strategic modifications, were we add an additional linkage to the chassis. This design refinement aims to address identified issues and enhance the overall structural integrity of the bike chassis. The subsequent round of modal and structural analyses using Ansys evaluates the effectiveness of these modifications. The results are compelling, showcasing a substantial reduction in deformation. Furthermore, the equivalent stress experienced by the chassis witnesses a significant decrease. These improvements overall the efficacy of the design modifications, resulting in positive impact on the structural performance of the bike chassis.

Keywords: Finite Element Method, Chasis Design, Modal and Structural analysis, FEA, Trellis Chasis.

ICRTMD-2023/ST/157 Development of Nano Bio Fertilizer via Chemical and Biological Synthesis

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Abstract

Achieving and maintaining optimal food security is a global task that initiates agricultural approaches to be revolutionized effectively on time, as adversities in climate change, population growth, and loss of arable land may increase. Recent approaches based on nanotechnology may improve in vivo nutrient delivery to ensure the distribution of nutrients precisely, as nanoengineered particles may improve crop growth and productivity. The underlying mechanistic processes are yet to be unlayered because in coming years, the major task may be to develop novel and efficient nutrient uses in agriculture with nutrient use efficiency (NUE) to acquire optimal crop yield with ecological biodiversity, sustainable agricultural production, and agricultural socio-economy. This study highlights the potential of nanofertilizers in agricultural crops for improved plant performance productivity in case subjected to abiotic stress conditions.

MOF-Engineered Janus Micromotors: Pioneering the Future of Antibiotic Waste Management

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Abstract

The rampant use of antibiotics has revolutionized modern medicine, enabling effective treatment against bacterial infections. However, this widespread use has inadvertently led to the emergence of antibiotic-resistant bacteria, posing a significant threat to global public health. To address this challenge, novel strategies for antibiotic degradation are urgently needed.

Janus micromotors, named after the two faced roman god, Janus, are a class of micro/nano scale particles with asymmetric properties, have emerged as promising candidates for antibiotic degradation. These self-propelled particles can navigate through aqueous environments and interact with antibiotics, facilitating their degradation. The unique characteristics of Janus micromotors, including their ability to generate motion and their tunable surface properties, offer several advantages for antibiotic degradation applications. Out of all the materials which have been employed for the fabrication of Janus micro motors, MOFs are the top choice due to their to their unique properties and tunable structure, high surface area and chemical stability.

One of the primary advantages of MOF based Janus micromotors lies in their ability to enhance mass transport. By generating motion, Janus micromotors can actively transport themselves towards antibiotic molecules, increasing the rate of encounter and degradation. This enhanced mass transport can significantly accelerate the degradation process, particularly in environments with low antibiotic concentrations. The degradation of antibiotics by Janus micromotors can be achieved through various mechanisms all of which generate ROS (Reactive Oxygen Species) which are highly capable of oxidising and breaking down the antibiotics. The utilization of MOF based Janus micromotors for antibiotic degradation offers several advantages over traditional treatment methods. Their self-propelling ability enhances their access to antibiotics, improving degradation efficiency. Additionally, they can be tailored with specific functionalities, such as magnetic or light control.

In conclusion, MOF based Janus micromotors represent a promising technology for the degradation of antibiotics in wastewater. Their self-propelling capabilities, combined with their ability to utilize various degradation mechanisms, make them a powerful tool for combating antibiotic resistance and safeguarding public health.

Keywords: Janus micromotors, MOF, antibiotic degradation, antibiotic resistance, environmental remediation.

Antimicrobial peptide-functionalized iron oxide nanocomposite for effective remediation against microorganisms

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Abstract

From rendering antibiotics and antimicrobial agents less effective to posing a much greater financial burden, antimicrobial resistance (AMR) is a global problem that has posed serious challenges in various biomedical sectors. Microbial resistance has even rendered antimicrobial peptides (AMPs) ineffective in recent times. The objective of this study was to formulate an AMP carrier model comprising a magnetic core modulated with chitosan as a platform for enhancing the antimicrobial propensities of Nisin. Remarkably, the N-CS-IONP nanoconjugates exhibited significantly greater antibacterial potency than the bare IONP and Nisin, with even Nisin-resistant Gram-negative bacteria becoming sensitive to nanomolar concentrations of the nanocomposite. The nanoconjugates even inhibited the biofilm significantly. Further investigation revealed that the enhanced antibacterial activity was linked to the elevated production of reactive oxygen species (ROS) at both the interfacial and intracellular levels. To summarize, the current study demonstrated that the adsorption of nisin at chitosan-coated IONP interfaces can significantly amplify its antibacterial potency against a wide range of bacteria, including those that are resistant to intact nisin. The IONP, CS-IONP, and N-CS-IONP nanocomposites were characterized by various biophysical techniques such as FTIR, SEM, XRD, DLS, and ZETA. The present study also addressed the effect of the components of nanocomposite primarily IONP and CS-IONP against HEK cellular viability.

Keywords: Magnetic Nanoparticles, Nanoconjugates, Antimicrobial resistance, ROS, Biofilm.

Design and fabrication of 23×15×11 CNC router machine for Milling

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Abstract

The current work's primary objectives are to investigate the theoretical and technological processes for designing, manufacturing, assembling, and testing electromechanical subsystems for creating a miniaturised, highly precise, and reasonably priced three-axis vertical CNC milling machine for quick prototype machining, small parts, and engraving small features in the electrical and medical industries, equipment should have an intuitive interface, high speed, low power consumption, durability, and safety. The goal of this research is to develop and construct a router machine using computer numerical control (CNC) that can grind pieces up to $23 \times 15 \times 11$ inches in size. The goal of this research is to assist traditional machine operators in increasing the output and efficiency of a company. To ensure accuracy and the router machine is operated by a stepper motor driver that moves the machine in three directions. The machine's workspace measured 23 inches by 15 inches by 11 inches. To achieve a more exact motion, the stepper motor is coupled with a ball screw on a linear bearing and powered by a Minebea Mitsumi PM stepping motor.

Formulation of an appropriate equation of state to predict the melting temperature of metallic solids

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Abstract

In our present work, we have found the pressure dependency of the melting temperature(Tmp) of metals using isothermal equation of state. The predicted models define the relation among the pressure, bulk modulus, melting temperature, volume compression and its first order pressure derivative at zero pressure. Then, the Tmp (K) of the metals Pt, Pd, Ni, Cr, Co, Au, Cu, Zn and Cd have been determined using different equation of state (Singh and Kao, Kholiya and Murnaghan). The melting temperature of metals increases non- linearly with the rising pressure. This study also shows a quantitative prediction of pressure on melting temperature of metals. Our obtained results using Singh And Kao EOS (Equation of state) show good agreement with the experimental data in comparison to other equation of State It is observered that Singh and Kao EOS is more capable to predict the melting temperature of metals for which there is no experimental data present.

Keywords: Thermodynamic, Volume compression, Bulk Modulus, Melting temperature, Thermal expansion.

ICRTMD-2023/ST/166

Modeling of the thermal conductivity of metal and metal oxide nanofluids with varying concentration

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Abstract

The thermal conductivity is one of the most relevant property of nanofluids (nfs). It is influenced by various factors such as shape, size, concentration, viscosity, temperature and Brownian motion. Nowadays, many models are present which explain the thermal conductivity of nanofluids but no model could explain the thermal conductivity of nanofluids but no model could explain the thermal conductivity of nanofluids properly. Using both the static and dynamic parameters of nanofluids, we proposed a model whose accuracy is more in comparison to other predefined models, such as Maxwell model, Hamilton-Crosser and Xuan model. We did some modification in Xuan model which gives the appropriate result closer to the experimental data in comparison to other model of metal and metal oxide nanofluids. We have tested our model for metal nanofluids like A1, Cu and metal oxide nanofluids TiO₂, SiO₂, WO₃. Our plotted graphs show good agreement with the experimental data using our proposed model. This shows that our proposed model will be more capable to predict the thermal conductivity for all the metal and metal oxide nanofluids for which there is no experimental data available.

Keywords: Thermal conductivity; Nanofluids; Concentration; Static and dynamic parameters; Xuan model.

ICRTMD-2023/ST/168

Thermodynamically Simulating Cool Thermal Energy Storage System (CTESS) with Encapsulation of Phase Change Material (PCM)

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Abstract

Maintaining persistence thermal effectiveness during charging of a Cool Thermal Energy Storage (CTES) system is challenging process. In this study CTES's thermal effectiveness has been examined with assimilation of packed bed mechanism in a cylinder capsules filled with phase-change material (PCM). A Numerical model is employed with assimilation of energy balance and Heat Transfer Fluid (HTF) equations. Temperature of PCM, total energy stored in the tank, solidified mass fraction of the tank and effect of mass flow rate of HTF is examine with various variables such as time frame (t=0 to 13.5hr) and mass fraction (mf = 1000 kg/hr), Kc = 0.15 - 2.5 Wm/K, ks = 2.22 - 3.2 Wm/K, diameter of the capsules (dc = 7.7 - 10 cm) and length of capsule (l = 1 dc to 4 dc). Flow rate of HTF and capsule's wall material and diameter are simulated for the complete solidification time of PCM, Energy stored in the tank and solidified mass fraction. Furthermore, the effect of thermal conductivity of PCM and length of capsule is examined on the energy storage and solidified mass fraction of the tank. It is concluded that the all examined parameters affects the performance of the latent heat storage system and proposed CTES is helpful in conserving heat energy and utilizing as the substitute of electric energy.

Keywords: Cool Thermal Energy Storage, Phase Change Material, Heat Transfer Fluid, Packed bed mechanism, Thermal conductivity.

ICRTMD-2023/ST/169 Finite Element Analysis of CFRP Composite Laminates with Ply- Discontinuities

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Abstract

In the present research work, a study has been conducted to understand the effect of ply – discontinuities on the strength of the Fiber Reinforced Polymeric Composite. FE Analysis for Four-Point Bend Test specimen has been carried out using ABAQUS software. Four different geometries having discontinuities at different locations have been considered for the present analysis.

Cohesive Zone Modeling is employed to simulate crack propagation pattern during failure of laminate. Present results from FE analyses have been validated with the experimental results available in literature. Results from FE analyses indicate that maximum stress concentration occurs at interface of resin pocket and discontinuous ply. Flexural strength of the considered laminate has been evaluated through FE analysis. Subsequently, failure process along with crack propagation pattern has been studied in detail.

Keywords: Composite material, Ply - Discontinuities, CFRP laminate, Cohesive Zone Modeling.

Unified model for the studies of band gap of nanosolids with their varying shape and size

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Abstract

Recent studies on the variation of band gap of nanoparticles with their shape and size has been a matter of great interest among the material scientists for tailoring of materials for their variety of applications. In the present work, we have studied the variation of band gap of low dimensional solids using modified cohesive energy band model with their varying shape and size of nanoparticles. It is observed that the complete consideration of shape, size, packing density, and unsaturated bonds of the surface atoms are missing in the various thermodynamical models, proposed by the earlier group of researchers. We have proposed a simple theoretical model for cohesive energy extending the bond energy model. In this model we have incorporated almost all the parameters required for providing a more thorough relationship between the band gap and nanoparticle characteristics. The band gap of the compound semiconducting nanoparticles, ZnX and CdX (X = S, Se, Te) have been calculated for different shapes. It has been observed that the band gap of nanoparticles increases when the particle size reduces, and the shape become more asymmetrical. Our calculated results show strong agreement with the available experimental data and the pre-defined theoretical models. Proposed model for the prediction of band gap of nanoparticles models. Proposed model for the prediction of band gap of nanoparticles increases when the particle size reduces, and the shape become more asymmetrical. Our calculated results show strong agreement with the available experimental data and the pre-defined theoretical models. Proposed model for the prediction of band gap of nanoparticles increases when the prediction of band gap of nanoparticles increases when the particle size reduces, and the shape become more asymmetrical. Our calculated results show strong agreement with the available experimental data and the pre-defined theoretical models. Proposed model for the prediction of band gap of nanoparticles may be useful for those materials for which

Keywords: Nanoparticles; Band gap; Cohesive energy; Packing density.

ICRTMD-2023/ST/172 Biocompatible and Targeted Nanocomposites for Enhanced Magnetic Resonance Imaging Applications: A Comprehensive Synthesis and Characterization Approach

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Abstract

Contrast agents are crucial in enhancing the visibility of internal structures during medical diagnosis, particularly in magnetic resonance imaging (MRI). Administered intravenously, these agents interact with the body's magnetic field, altering the signal strength of specific tissues or organs, enabling clearer delineation and improved diagnostic capabilities. Gadolinium-based contrast agents (GBCAs) have long been the main stay of MRI contrast enhancement, providing significant improvements in image quality. However, safety concerns have emerged, prompting the search for alternative agents that maintain efficacy while mitigating potential adverse effects. The advent of nanotechnology has opened up new avenues for developing innovative contrast agents with tailored properties. A promising approach involves the design of multifunctional nanoparticles that incorporate a metal ion, an organic ligand, and a targeting moiety. The metal ion, such as manganese, iron, and other transition metal, can serve as the core contrast-enhancing element, while the organic ligand stabilizes the metal ion and enhances its biocompatibility. The targeting moiety, a specific molecule that binds to a particular disease marker, enables selective accumulation of the nanoparticle at the desired site of action. This targeted delivery not only improves image specificity but also reduces the overall dose of contrast agent required, minimizing potential side effects. The proposed three-dimensional structure of these multifunctional nanoparticles offers several advantages over traditional contrast agents. The organic ligand effectively reduces the toxicity of the metal ion, a major concern with GBCAs. Additionally, the nanoparticle structure allows for incorporation of multiple contrast-enhancing units, potentially enhancing signal intensity and reducing the overall dose required. Moreover, the incorporation of a targeting moiety endows the nanoparticle with the ability to specifically target diseased tissues, leading to improved image contrast and reduced systemic distribution of the contrast agent. This targeted approach holds promise for enhancing the diagnostic accuracy of MRI while minimizing potential adverse effects.

Keywords: MRI contrast agent, nanomedicine, MOF, biocompatibility, nanocomposites.

Investigation on the optical, dielectric properties and AC conductivity of PVA/PVP/ZnO blend based polymer nanocomposites for optoelectronic and electronic device applications

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Abstract

Polyvinyl alcohol/Polyvinyl pyrrolidone/Zinc oxide (PVA/PVP/ZnO) nanocomposites for different weight percentages of ZnO nanoparticles (0, 5, 10, 15 and 20 wt%) has been prepared by solution casting method. XRD and EDX results confirmed the polymer nanocomposites formation and purity of the samples. An increase in roughness of the polymer nanocomposites by the addition of ZnO is evident from the AFM images. FTIR analysis confirmed the physical interaction between the hydroxyl group of PVA, carbonyl group of PVP and ZnO nanoparticles. The band gap energy decreases from 5.30 eV to 2.10 eV with increasing ZnO nanoparticles content in the PVA/PVP blend matrix. The nanocomposites showed zero transmittance in the UV region suggesting that the nanocomposites could be used as a potential UV shielding material. The dielectric constant values of these nanocomposites are found in the range 14-23 with dielectric loss value of 0.09. The conduction mechanism observed in AC conductivity for all samples is governed by small polaron tunnelling model (SPTM). These properties of PVA/PVP/ZnO nanocomposites suggests their suitability for use as an insulator in the fabrication of micro electronic device applications.

Keywords: Polyvinyl alcohol/Polyvinyl pyrrolidone/Zinc Oxide (PVA/PVP/ZnO), nanocomposites, XRD, band gap energy, dielectric, AC conductivity.

ICRTMD-2023/ST/175 Enhanced degradation of Congo-red dye by La³⁺ doped Fe₂O₃ nanoparticles under sunlight

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Abstract

Progress of nanocomposites for the effectual result in the removal of hazardous pollutants are always in demand due to increase in water pollution. In the present work α -Fe₂O₃ and La doped α -Fe₂O₃ nanoparticles were synthesized via hydrothermal route and used for the removal of congo-red dye present in industrial waste by adsorption property of developed material. XRD, FESEM, FTIR characterizations were performed to study the effect of Lanthanum doping in α -Fe₂O₃ on the degradation property. This study shows the tremendous adsorption ability of synthesized nanoparticles towards congo-red dye under normal sunlight in a short duration of 5 mins, which was further confirmed by UV spectroscopy. The results showed the degradation rate of α -Fe₂O₃ is 52.3% after 5 mins which increases extraordinarily to the degradation rate of 99% by doping of Lanthanum. Our findings specify that the La doped α -Fe₂O3 synthesized nanomaterial has a great potential for the removal of dye from industrial waste like Congo-red from pollutants.



Fig: UV-visible absorption spectroscopy of LaFeO₃.

Keywords: Nanoparticles, degradation, adsorption, pollutants

Preparation of Ficus religiosa leaves extract and its applications in green synthesis of zinc oxide nanoparticles and antimicrobial activity

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Abstract

This study reports the synthesis of ZnO nanoparticles using the aqueous solution of peepal leaves (Ficus religiosa leaves) extract. The nanoparticles, represented as Peep-ZnO (with broccoli extract), were obtained after calcination. The nanoparticles were characterized using X-ray diffraction (XRD), UV-visible Spectrophotometry (UV-Vis), and Fourier Transform Infrared Spectrometer (FTIR). Nanoparticle amalgamation via green routes is a well-established technique that gives rise to nanodimensional materials that are convenient, and their utility is essential in various fields where eco-friendly stuff is the need of the hour. The primary study is a cost-effective, environment-friendly, and straightforward technique to prepare zinc oxide nanoparticles (ZnONPs) using Ficus religiosa leaf extract.

Zinc nanoparticle green synthesis is most widely used in the medical field, food preservation, the textile sector, textile coatings, and other environmental uses. At non-cytotoxic doses, antiviral activity of zinc nanoparticles against HIV-1 has been demonstrated. Zn NP has already been studied and found to exhibit promising antibacterial activity. However, most of the methods for the production of nanoparticles involve various hazardous chemicals and harmful byproducts. Consequently, it's crucial to identify ZnO NP as a common antibacterial agent in the healthcare sector, food storage, textile coatings, and numerous environmental applications. In this work, the antibacterial property of the Peep-ZnO particles was inspected, and the results showed the prepared particles as promising antibacterial agents.

Keywords: Ficus religiosa, leaf extract, nanoparticle, ZnO.

ICRTMD-2023/ST/180

Structural, Electronic and RDG Analysis on Cadmium Chloride Adipic Acid by DFT Approach

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Abstract

In order to obtain the geometry of the molecule Cadmium Chloride Adipic Acid (CCAA), computational procedures were carried out utilizing B3PW91 with LANL2DZ basis set extending Gaussian'09W program. Charge transmission within the molecule is demonstrated by the computed HOMO and LUMO energies. Their chemical reactivity has been further explained by the calculation of several reactivity parameters. The more accurate measure of global chemical reactivity is the global electrophilicity index, whose value of 6.18676 eV characterizes the biological activity of the substance in question. Using RDG analysis, the interactions inside the CCAA molecule were examined.



Study of Thermal Expansion Coefficient of Nanomaterials using different equation of state with varying Shape and Size

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Abstract

N a n om a te ria ls, ow in g to the ir u n iqu e siz e a n d sh a p e d ep en d e n t p ro p e rties, p re sen t a fa sc in a tin g a ve n u e for re sea rch in th e w orld of m a te ria ls scien c e. T h is stud y system a tic a lly in v estig a tes th e d iffere nt th e rm od yn a m ic p a ra m eters d e p en d en c y o n n a n om a terials, sp ec ially on th erm al e xp a n sio n , vo lu m e c om p ressio n v a ria tion s, a n d b u lk m o d u lu s. W e h a v e stu d ie d th erm o d yn a m ic p a ra m e ters of n a n om a teria ls u sin g tw o eq u a tio n of state s th at is U su a l-T a its E O S a n d K h o liya E O S .T h e te m p era tu re flu ctu a tio n a nd vo lu m e c om p ressio n for d if feren t sh a p e s o f n a n om a teria ls.T h e p re d e fin e d ex p e rim en ta l d a ta is c om p a red w ith th e o u tc om es p rod u ce d b y th e cu rre n t m od el. T h e a cc u ra c y of th e cu rren t m od el for ex am in in g th e th e rm a l ch a ra cteristic s of n a n om a terials is con f irm ed b y th e h ig h a g re em en t b e tw e en th e co m p a red resu lts. Keywords:

N a n om a te ria l; siz e e ffec t; th erm a l e xp an sio n ; e qu a tio n of sta te s

ICRTMD-2023/ST/191 Synthesis and Characterization of Mn0.5Zn0.5Fe2O4 mixed ferrite nanocomposites with CNT

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Abstract

Ferrites have garnered significant attention in recent years due to their exceptional structural, magnetic and optical properties. This heightened interest is reflected in their diverse applications ranging from dye degradation and energy storage to sensors and drug delivery. In this work, manganese-zinc mixed ferrite with composition $Mn_{0.5}Zn_{0.5}Fe_2O_4$ was synthesized using the chemical co-precipitation method. The nanocomposites of synthesized mixed ferrite nanoparticles with different compositions of CNT (2%, 4% and 6%) were made using the ultrasonication method. The prepared samples were characterized by using different techniques. The structural analysis using X-ray diffraction (XRD) confirmed the formation of a single spinel phase cubic spinel structure. Fourier transform infra-red spectroscopy (FT-IR) confirmed the presence of bonds associated with spinel structures. HRTEM revealed a homogenous dispersion of CNTs indicating effective interfacial interaction with the ferrite nanoparticles. Magnetic properties were assessed through vibrating sample magnetometry (VSM) showcasing an increase in saturation magnetization with the inclusion of CNTs. In conclusion, the integration of carbon nanotubes into manganese zinc mixed ferrite nanocomposites has been successfully achieved, leading to enhancement in various properties such as the structural and magnetic properties. This study contributes valuable insights into tailoring nanomaterials for advanced applications opening avenues for the development of high- performance materials.

Keywords: Ferrites, Carbon Nanotubes, Chemical Co-precipitation, Ultrasonication method, XRD.

ICRTMD-2023/ST/192

Applications of the platinum nanoparticle for Sensitively and Selectively Determination of lead ions using square wave Voltammetry

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Abstract

Most heavy metal ions are carcinogenic when present in high amounts, therefore its reliable, rapid and on-site detection is crucial. Square wave voltammetry (SWV) is a powerful electrochemical technique that offers high sensitivity and selectivity for the detection of heavy metals, including Pb^{2+} ions, therefore, in the present study, Square Wave Voltammetry technique applied in conjunction with noble metal platinum nanoparticles (Pt NPs) for the detection of lead ions. PtNPs-modified electrodes have demonstrated remarkable performance in the detection of Pb^{2+} , offered low detection limit - 0.046 μ M, high sensitivity - 42.195 μ A μ M⁻¹, linear range - 0.1 to 0.5 μ M, and regression coefficient – 0.95, respectively, making it promising candidates for real-time monitoring of Pb^{2+} contamination in environment. The proposed sensor was also tested on the tap water to check the cross-sensitivity and it was found that no interference occurred for real water sampling. Furthermore, the outcomes of this investigation demonstrated high repeatability. As per the findings of these outstanding results, the proposed sensor (PtNPs) is highly sensitive and can detect lead ions concentrations as low as 0.04 micromolar (10⁻⁶ moles per litre), that is much lower than the concentration of lead ions considered to be safe for humans.

Keywords: Platinum Nanoparticles, Sensor, Lead, Electrochemistry, Square Wave Voltammetry, Sensitivity.

An Outstanding electrochemical behavior of plasma exposed activated carbon derived cotton stalk

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Abstract

Biomass materials were widely used to synthesize the porous carbon for energy storage's while considering the simple preparation method and wide availability of raw material. The temperature has a significant impact on the surface area and pore structure of activated carbon, which in turn affects the material's capacitive performance when derived from biomass waste materials. Here in activated carbon was made from cotton stalk using the pyrolysis method. It is one of the low-cost method of carbon production in order to achieve their widespread applications. The Activated cotton stalk carbon (ACCS) was exposed to DC glow discharge plasma with an applied potential of 450 V and the pressure of 0.3mbwas used to enhance the surface properties. The XRD, FTIR, FESEM and Raman were utilized to analysis the crystalline nature and surface properties of plasma treated and untreated ACCS. The electrochemical behavior of untreated and plasma treated ACCS was investigated using three electrode methods. With these experimental conditions, the two different electrolytes KOH and NaOH was investigated, the ACCS shows an excellent electrochemical characteristics in KOH electrolyte. The results demonstrated that the plasma treated ACCS electrode performs better than the untreated electrode. The outline of the research reals that, the plasma treated porous carbon electrode made from waste biomass cotton stalk is suitable for high-performance supercapacitors.

Keywords: Activation temperature; Cotton stalk; Supercapacitor; pore structure; Electrode.

Study of Zone Center Phonons in Double Perovskite Oxides

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Abstract

The investigation employed a short-range force constant model to analyze Raman and infrared phonons within the tetragonal structure of the double perovskite, characterized by space group I4/m. Utilizing six stretching and three bending force constants, this study conducted theoretical calculations of zone center phonons through normal coordinate analysis. The frequencies determined in this research align well with experimentally observed frequencies. Additionally, an exploration of potential energy distributions (PED) delves into the influence of interatomic forces on the calculated Raman and infrared phonons for these compounds.

Keywords: Double Perovskite, Phonon, Raman Wave number, Infrared Wave number.

Probing external factors in Advanced Glycation Endproducts driven metal nanoparticle synthesis for development of a sensing system

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Abstract

Chemical reactions between sugars and the available amino groups on proteins, lipids, and nucleic acids lead to molecular malfunction by creating advanced glycation end products (AGE). AGE have adverse effects on a broad spectrum of chemical, cellular, and tissue scale through alterations in charge, solubility, and shape that define molecular senescence. Individuals with diabetes are susceptible to chronic issues, such as cataract, retinal disease, hardening of the arteries, nerve damage, kidney disease, and hindered healing of wounds. In our work, we have developed metal nanoparticles which can be synthesized with in-vitro genesis of AGEs from hemoglobin. These extremely responsive hemoglobin derived AGEs are able to reduce gold and silver ions to create gold (AuNP) and silver nanoparticles (AgNP) with a distinct plasmonic reaction compared to the control solutions. In order to enhance comprehension of the contrast between AuNPs and AgNPs, a comparative analysis has been conducted by distinguishing external factors. The metal nanoparticles were observed over a period of time and it was determined that the AuNPs remain stable and exhibit excellent colloidal stability. However, when AgNPs were synthesized using AGE derived from hemoglobin, they were found to be unstable. Thus, in this work we have optimized the optical properties of both the metal nanoparticles in terms of synthesis, influencing factors and stability for development of AGE sensors as a futuristic goal.

Keywords: Advanced glycation end products (AGEs); Sensor; Hemoglobin; Nanoparticles; Plasmon.
Investigation of adsorption efficiencies of graphene oxide and graphene oxide Montmorillonite composite for the removal of organic dye

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Abstract

In this work, Graphene oxide (GO) and Graphene oxide-montmorillonite (GO-Mt) composite was successfully synthesized and used for the removal of cationic dye, Malachite green dye. X-ray diffraction (XRD) and Fourier transform infrared (FTIR) spectroscopy were used to study the novelty in the structural characterization of these composites. Furthermore, Graphene oxide and Graphene oxide-montmorillonite composite are used as an adsorbent for the removal of dye through batch extraction as a function of pH, contact time and concentration. UV Visible spectroscopy was used to determine the pH stability of Malachite oxalate green (MG) dye which indicates that malachite oxalate green dye is not stable at any pH. XRD results indicated successful formation of an exfoliated structure in the composites. The disappearance of peak at $2\theta = 8.1^{\circ}$ were observed for montmorillonite, indicating the homogenous distribution of the GO sheets into the activated clay structure. The maximum uptake of Malachite green dye with Graphene oxide-montmorillonite (GO-Mt) composite was 675 mg/g at pH 8 within 150 minutes of contact time is more efficient than the graphene oxide composite which absorb 318.88 mg/g at pH 8 within 30 minutes of contact time. The adsorption of dye was facilitated by functional groups that contained O and C. Additionally, the hydrophobic interaction between GO and MG, hydrogen bonds, and π - π and n- π interactions all played a significant role in adsorption. Therefore, the study showed that Graphene oxide-montmorillonite is great effectiveness and outstanding reusability, it may prove to be a promising and reasonably priced sorbent for the treatment of Malachite green dye.

Keywords: Graphene oxide, Malachite Green, Montmorillonite, Batch Extraction, UV-Visible Spectroscopy.

Polymer Nanohybrid as Efficient Heat Dissipation Material for Effective Cooling Applications

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Abstract

In today's technologically advanced world, there is a rapid emergence of energy-savings and energy-producing methods. Cooling plays a crucial role in various fields such as engines, electronics, and manufacturing by effectively reducing energy losses. To meet the growing demand for efficient coolant, new products and technologies are continuously being developed. While water is the most commonly used coolant, alternative combinations and systems have been developed over the past two decades to overcome its limitations. A highly efficient cooling system is necessary to improve current heat management systems and meet the cooling demands of advanced engine and electronic systems. The water based nanocoolant have been developed, wherein the nanoparticles used are polymer-carbon nanostructure hybrid material. The advantage of using hybrid material is the developed nanofluid have enhanced dispersion stability hence enhanced cooling properties. The nanofluids based on carbon nanomaterials e.g.; carbon nanotube (CNT), carbon nanofibers, graphene was prepared. A polymer-carbon nanostructure hybrid material was used in water based fluids. The dispersion stability of nanofluids was studied by varying the concentration of nanoparticles and best optimized concentration obtained was 0.1%. Carbon nanomaterial was taken for final nanofluids prepration and the base fluid taken was water. Two types of water soluble polymer were used, to coat the carbon nanomaterial viz; polyvinylalcohol (PVA) and polyvinylpyrrolidone (PVP). The effect of nanoparticles on enhancement of thermal conductivity of different nanofluids was studied using KD-2 pro thermal property analyzer. The polyvinylpyrrolidone (PVP) based fluids show higher enhancement in thermal conductivity than polyvinylalcohol (PVA) based nanofluids. Similarly when the effect of nanofluids was studied the graphenes based nanofluid shows higher thermal conductivity than carbon nanotubes based. The carbon nanotubes based nanofluid show higher enhancement in thermal conductivity than carbon nanofibers. A similar trend is observed in for both polymer based nanofluids.

Keywords: Polyvinylalcohol, polyvinylpyrrolidone, graphene, carbon nanotube.

Unraveling the Cosmos: A Comprehensive Study of General Relativity and its Profound Implications

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Abstract

Initiating a captivating exploration, the profound implications of general relativity, a revolutionary theory conceived by Albert Einstein in 1915, come to the forefront, reshaping our understanding of gravity. The journey unfolds with an exploration of the theory's foundational principles, traversing the intricate landscapes of spacetime curvature and the Einstein field equations. Through a lens of experimental confirmations, from the bending of light to the verification of gravitational waves, we witness the theory's empirical triumphs. Astrophysical implications come to the forefront, revealing the influence of general relativity on phenomena like black holes, gravitational lensing, and the expanding cosmos. A survey of alternative theories and ongoing debates underscores the continuing evolution of gravitational understanding. Applications of general relativity in technology and its role in shaping our universe's large-scale structure highlight the theory's practical relevance. As we delve into the lives of notable figures who contributed to its development, we emerge in the landscape of current research and future trajectories, witnessing the ongoing quest to unravel the deepest mysteries of gravity. This paper presented a comprehensive guide, weaving together historical context, theoretical underpinnings, astrophysical ramifications, and the latest advancements, inviting readers to embark on a captivating odyssey through the gravitational wonders of the cosmos.

Keywords: General Relativity; Einstein's Legacy; Astrophysical Insights; Gravitational Advancements.

ICRTMD-2023/ST/207 Synthesis, Characterization and Application of GdMnFe₂O₄ as an Advanced Humidity Sensor

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Abstract

Gadolinium-doped manganese ferrite (GdMnFe₂O₄) has emerged as a promising material for a wide range of applications due to its unique combination of humidity. This study explores the synergistic potential unlocked by gadolinium doping in manganese ferrite, specifically focusing on its implications for humidity sensing. The humidity sensing capabilities of Gd-MnFe₂O₄ were evaluated through resistance measurement, revealing a significant improvement in sensitivity and response time compared to undoped manganese ferrite. The introduction of gadolinium ions into the crystal lattice resulted in enhanced water vapor adsorption, leading to a more pronounced change in resistance with varying humidity levels. This unique sensitivity makes GdMnFe₂O₄ an ideal candidate for humidity sensing applications, such as environmental monitoring and industrial processes.

Keywords: Nanomaterials; Adsorption; Humidity; Sensor; Response time.

ICRTMD-2023/ST/214 Multifunctional Polymer supported Bimetallic Catalyst towards CO₂ Utilisation, Organic Synthesis and Environmental Aspects

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Abstract

Herein seven diverse application was evaluated using single heterogeneous material. The state-of-the-art of the composite, graphitic carbon nitride supported bimetallic catalyst, $g-C_3N_4/Ca^Ag$, for CO₂ valorization, organic synthesis, transformation, and environmental remediation to examine the power of this multifunctional catalyst. The sustainable chemistry of CO₂ valorization involving cyclisation of propargylic alcohols, and carboxylation of terminal alkynes and organic reactions associate three-component coupling, and Knoevenagel condensation, and reductive transformation of environmental pollutant and bacterial inhibition are performed. Most of the reactions withstand distinct moieties at good to better yields under benign reaction and solvent free conditions. The chemical, microscopic, and structural characterizations disclose that metallic Ag, and CaO with well-defined nanostructures are integrated on the $g-C_3N_4$ support. The polymeric conjugated metallic centers work synergistically on a platform with moderate surface area and good CO₂ adsorption capacity for emerging green sustainable heterogeneous catalysts.

Keywords: heterogeneous catalysis; spectroscopy; CO₂ valorization; organic synthesis; transformation; environmental remediation.

Nanoencapsulation of Cymbopogon nardus essential oil and their bioactive constituents: A novel strategy to control mycotoxin contamination in the food system

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Abstract

The essential oil has been tested against a wide range of foodborne fungi and its associated mycotoxins. The present study explores the enhanced antifungal, aflatoxin B₁ (AFB₁) inhibitory activity and lipid peroxidation efficacy of Cymbopogon nardus essential oil encapsulated in chitosan nanomatrix (CNEO-CSNPs) against a toxigenic strain, Aspergillus flavus. Ionic gelation method was used to synthesize CNEO-CSNPs were characterized using DLS, Zeta potential, FTIR, XRD, and TEM instruments and tested for enhanced biological activity. In-vitro assessment, 0.75 μ L/mL of CNEO-CSNPS absolutely restrain the development of A. flavus while preventing the production of AFB₁ at 0.50 μ L/mL in comparison with pure CNEO. According to the biochemical mode of action, CNEO-CSNPs significantly suppressed ergosterol, ions leakage, mitochondrial membrane potential, and the antioxidant system. Similarly, in-situ trials on A. hypogea seeds with CNEO-CSNPs prevented fungal proliferation, AFB1 production, and lipid peroxidation without damaging the seed germination. The present study revealed that CNEO-CSNPs might be encouraged as a potential environmentally green preservative against food pathogens and to enhance food product shelf life.

Keywords: Antifungal; Mode of action; Cymbopogon nardus oil; Chitosan; Nanoencapsulation.

ICRTMD-2023/ST/224 Study of Thermal Conductivity of Metallic Nanoparticles varing shape and size

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Abstract

Thermal conductivity of metallic nanoparticle has garnered significant attention due to its potential application in various fields including electronics, materials science and energy. This abstract provides a concise overview of key aspects related to the thermal conductivity of metallic nanoparticle .In our work, we have studied the Thermal Conductivity of Metallic Nanoparticle with the variation of different size and shape factor. We have also proposed a model to predict the change in Thermal conductivity varing shape and size. It has been observed that the Thermal Conductivity of Metallic Nanoparticle decreases by lowering the size of Nanoparticle. It has been found the computated value has a maximum deviation $\pm 7\%$ with experimental results which is under permissible range of experimental data.

Keywords: Metallic.Nanoparticles, thermal conductivity, size effect, shape effect.

Coordination Between Recyclers and Pollution Control Board

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Abstract

Apart from the level of awareness, coordination between the recyclers and respective state authorities plays a prime role towards formal e-waste management system. Coordination between the recyclers and state boards were analyzed using One-way ANOVA and found that there is a lack of coordination and effectiveness between the two. It was also found that there is no difference in the opinion of different areas of recyclers when tested with the questionnaire.

Keywords: E-waste, Management, Recycling, Recyclers, State boards.

Animation & Cartoons as learning tools in Physics: A perspective

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Abstract

This exploratory study examines physics teachers' views of the effect of animations & cartoons on learning and teaching Physics. A 25-item survey questionnaire was distributed to 50 Physics teachers. The questionnaire comprised of two main constructs: a) Positive Effects of animations & cartoon on learning and b) Positive Effects of animations & cartoon on teaching. Findings showed that more than 70 per cent of the respondents have positive views on the impact of animations & cartoons on teaching and learning. Teachers view that teaching and learning using cartoons can create positive learning environment for the students and are able to stimulate students' imagination and creativity.

Keywords: Innovative teaching; Cartoon; Physics; Perceptions, Secondary teachers.

Bandwidth Enhancement of Microstrip Array Antenna using Gap Coupled Parasitic Patches

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Abstract

This study investigates a novel method for adding gap-coupled parasitic patches to microstrip array antennas to increase their bandwidth. Because of their small size and directed radiation qualities, microstrip array antennas are widely used in many communication systems. Nevertheless, it is frequently difficult for them to match the expectations of contemporary communication applications due to their low bandwidth. The method suggested in this paper is adding thoughtfully crafted parasitic patches to the microstrip array structure, with gaps set at suitable intervals. The gap-coupled parasitic patches are essential for adjusting the current distribution and impedance matching, which widens the antenna bandwidth. Utilizing cutting-edge electromagnetic simulation tools, the study optimizes the parasitic patches' geometric parameters and examines how they affect the antenna's overall performance. The proposed improvements to a prototype microstrip array antenna are fabricated and tested to validate theoretical insights through practical experimentation. Findings show that the antenna's bandwidth has significantly improved, which qualifies it for uses that call for higher data rates and improved communication capabilities. The results of this study provide important new information for the continuing efforts to create effective and small antenna systems for contemporary communication technologies.

Keywords: Bandwidth enhancement, Gap coupled parasitic patches, Microstrip array antenna.

Effect of Fe dopant on ZnS nanoparticles synthesized from solid-state reaction

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Abstract

The present research is focused on the synthesis and characterization study of pure and Fe-doped zinc sulfide (ZnS) nanoparticles using an inexpensive method i.e., solid-state reaction process. The XRD patterns showed that the structure of nanoparticles is a cubic zinc blend. The presence of zinc, sulfur and iron in the samples was verified by EDAX analysis. The formation of spherical-shaped clusters was confirmed by FE-SEM images. Absorption ranges and energy band gaps were investigated by UV–Vis spectroscopy. The investigation of photoluminescence spectra reveals the dopant incorporation into the ZnS structure. The XPS (X-ray spectroscopic) studies confirmed that the presence of Fe²⁺ ions in host ZnS nanoparticles.

Keywords: Nanoparticles, Cubic zinc blend, Crystal structure, Photoluminescence, XPS.

Morphological and Optical Studies of Hydrothermally Synthesized NiO/NiS Nanocomposite

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Abstract

The present work focuses on the modification of band gap of nickel oxide/nickel sulfide (NiO/NiS) nanocomposites, paving the way for future solar cells that are not only high-performance but also cost-effective, thereby promoting broader adoption of sustainable energy sources. The NiO/NiS nanocomposites were synthesized using a one-step hydrothermal route. The X-ray diffraction (XRD) pattern revealed the phases of NiS and NiO. Crystallite size and strain for the as synthesized material was calculated using techniques like Debye Scherrer Size-Strain plot and Williamson-Hall analysis. UV-visible spectroscopy revealed optical band gap of as synthesized material near 1.3eV. The absorption spectra revealed the material to suitable for solar applications. Field emission scanning electron microscopy (FESEM) was applied to study the morphological characteristics of the particles, which showed that the nanoparticles have a hexagonal structure. Energy dispersive spectroscopy (EDS) was also used for elemental analysis, showing the presence of sulfur, oxygen, and nickel.

Keywords: Hydrothermal, Nickel oxide, Nickel sulfide, Hexagonal crystal structure, Optical band gap, Nanocomposite.

Morphological and Optical Analysis of Tungsten Oxide Nanosheets for Gas Sensing Application

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Abstract

Tungsten oxide (WO_3) is a well-known transition metal oxide that exhibits non-toxicity and stability in its nanoparticle form. It is a potential candidate for a variety of applications due to its low cost and facile synthesis process. In the present work, WO_3 nanoparticles have been synthesized via one-step hydrothermal route. X-ray diffraction pattern revealed the formation of a single phase tungsten trioxide with high crystallinity. The average of analysed peaks was determined to calculate the crystallite size of tungsten trioxide (WO3) which is found to be 23.15 nm. Crystallite size and strain were used to explain the structural defects and formation mechanism of WO_3 . UV- visible spectroscopy was utilized to study the optical properties, resulting in a band gap of 2.56 eV in the single phase of WO_3 . Scanning electron microscope (SEM) images demonstrated the morphological properties of material. As a result, tungsten trioxide was found to be more environmentally sensitive than pre-transition-metal oxides.

Keywords: Tungsten oxide (WO₃), Metal oxide, Nanoparticles, Nanosheets.

Numerical Modelling and Simulation of Phase change material Melting

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Abstract

In this paper we have done a comprehensive examination and simulation of the melting process of a Phase Change Material (PCM) for thermal energy storage. The simulation encompasses the gradual melting of a rectangular domain of size (150mm * 100mm) composed of PCM.For the sake of simplicity, we have taken paraffin wax as PCM for our simulation process. This domain features its left side subjected to a consistent heat flux of 2500 W/m², while the remaining three sides remain thermally insulated i.e in adiabatic conditions. In this specific case with a vertically oriented heating wall, the melting process initiates at the upper portion of the PCM domain and subsequently proceeds in a downward direction. We also observed a time dependent behaviour of matrial in melting process, i.e., in the initial stages it remained relatively consistent but as soon as the advancement in time occurred the rate of melting also increased, this increased rate is most noticeable from middle of the melting process. The entire simulation is executed through the utilization of the ANSYS (Fluent) 23.0 software platform. The paper also delves into the elucidation of the underlying assumptions, the formulation of equations employed in the numerical modelling process, and a thorough delineation of the software's specifications. Additionally, the paper provides a comprehensive depiction of various contours, including those representing liquid fraction, density, temperature, and particle velocity of the PCM. These contours are presented at regular intervals, with a cadence of 30 minutes, over the course of a total melting duration spanning 240 minutes (equivalent to 4 hours). The contours serve as instrumental tools for discerning and elucidating alterations in the melting interface's shape and motion as time progresses. Furthermore, the paper delves into an in-depth exploration of the temporal evolution of the melting fraction. This provides valuable insights into the percentage of PCM that has undergone melting at distinct time intervals. This paper also underscores the importance of proper meshing and selection of appropriate time steps when simulating melting problems in ansys(fluent). Inadequete meshing and selection of improper time steps can lead to divergence errors during solution phase.

Keywords: Phase change materials, GHG, Thermal energy storage, Latent heat storage, CFD.

CTAB-Assisted Hydrothermal Synthesis of MoO₃ Nanoparticles: Multifaceted Characterization and Analysis

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Abstract

Molybdenum Oxide (MoO₃) is a wide-gap n-type semiconductor that is exceptional in catalytic, optical, and electrochemical applications. It has received a lot of fascination from both fundamental research and real-world applications. In the present work, monoclinic phase MoO₃ has been synthesized by hydrothermal route and the effect of CTAB surfactant on the properties of MoO3 has been studied. The as-synthesized material exhibits the crystallite size of approximately 42 nm. The crystallite size was determined by using Debye-Scherrer equation, Williamson-Hall plot, and size-strain plot. These analyses provided valuable insights into the structural properties of the material. The material demonstrated optical band gap of 3 eV, indicative of its semiconducting nature. UV-vis absorption spectroscopy revealed absorption exclusively in the UV region, aligning with its semiconducting properties. The exclusive UV absorption suggests potential applications in UV-sensitive devices. Field emission scanning electron microscopy (FESEM) analysis uncovered the morphology of MoO3, showcasing a distinctive array of nanorods and nanosheets. This morphological diversity is essential for understanding the material's structural intricacies, paving the way for tailored applications in various fields like Thin-Film Transistors (TFTs), Photodetectors, Solar Cells, Gas Sensors, Lithium-Ion Batteries, Fireproofing, Ceramic and Glass Industry, Water purification.

Keywords: Molybdenum Oxide, Cetyltrimethyl Ammonium Bromide (CTAB), Hydrothermal.

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Abstract

This study explores the distinct structural, morphological, and functional features of a range of perovskite oxide materials by fabricating and characterizing them. Perovskite oxides have attracted much attention lately because of their many uses in energy storage systems, electronics, and catalysis. The research utilizes an all-encompassing methodology, integrating diverse production techniques like sol-gel synthesis, hydrothermal procedures, and solid-state processes to customize the composition and structure of the examined perovskite oxides. To clarify the crystallographic, morphological, and chemical properties of the synthesized materials, a variety of detailed characterization techniques are used, such as Fourier-transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and X-ray diffraction (XRD). In addition, the study looks into the perovskite oxides' electrical, magnetic, and catalytic characteristics, offering important new information about possible uses in energy- and electronics-related devices. The study's results add to the expanding body of information about perovskite oxide materials and provide a basis for more investigation and property optimization for cutting-edge technology uses. Perovskite oxides' adaptability and tuneability highlight their potential to solve present problems and open the door for the creation of functional materials for the next generation.

Keywords: Perovskite oxides, Fabrication, Characterization, Structural properties, Functional properties.

Synthesis, Characterisation and Computational study of Meldrum acid Chalcone Derivatives by using green base

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Abstract

The synthesis of Meldrum acid chalcone by using green base The current inspection agreements with a detailed investigation on the computational study of Meldrum acid chalcone derivatives by using density functional theory (DFT). The enlarged molecular geometry, bond lengths, bond angles, atomic charges of the titled compound has been investigated by Density Functional Theory (DFT) using standard B3LYP method with 3-21+ G basis set using Gaussian 16 W package. The HOMO to LUMO transition implies an electron density transfer.

Keywords: Meldrum acid; DFT calculation; Mulliken Charge; HOMO- LUMO study; Chalcone.

Hydrothermal Synthesis and Characterization of Tin Telluride

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Abstract

Two-dimensional (2D) transition metal monochalcogenides have earned notable attention because of their distinctive electronic, physical, and chemical attributes. These materials find vast array of applications in energy generation, thermoelectric devices and gas sensing technology. Among these, tin telluride (SnTe), a member of the transition metal monochalcogenides, stands out for its remarkable qualities, featuring a narrow band gap and an environment-friendly, non-toxic nature. Prior research has demonstrated that the properties of SnTe can be effectively modified through the introduction of hydrazine during the synthesis process, resulting in enhanced conductivity and heightened sensitivity to environmental changes. Consequently, SnTe has captured the interest of researchers, particularly for its gas-sensing potential. In the current study, a facile hydrothermal method was employed to synthesize SnTe and conducted an in-depth analysis of its structural, and morphological characteristics through various characterization techniques. X-ray diffraction (XRD) analysis confirmed the formation of SnTe with a cubic crystal structure, revealing a crystallite size of 67.80 nm and strain 0.00200 using the Debye Scherrer equation. Additionally, UV-Vis spectrophotometer was employed to determine the absorbance plot and band gap of the synthesized SnTe sample. The hydrothermal synthesis process yielded SnTe structures with a distinctive spherical shape, as confirmed by field emission scanning electron microscopy (FESEM). In this study, non-toxic precursors and solvents, such as SnCl₂·2H2O, TeO₂, hydrazine, and ethylenediamine, were employed. Using these chemicals, SnTe was successfully synthesized through a straightforward and cost-effective hydrothermal method. In this work, SnTe having a direct and narrow band gap (0.18eV) was synthesized, which has potential applications in fields such as infrared detection, thermoelectric materials, and gas sensing devices. This technique provides a fundamental approach to manufacturing SnTe semiconductors. Tin telluride, as a group IV-VI semiconductor, holds significant promise for future research.

Keywords: SnTe, Narrow band gap, Monochalcogenides, Hydrothermal

Activated Charcoal for the Elimination of Methylene Blue Dye from Aqueous

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Abstract

The creation of activated carbon (AC) from raw charcoal is described in this paper. It takes one hour at a low temperature. X-ray diffraction (XRD), Raman spectroscopy, Fourier-transform infrared spectroscopy (FTIR), UV-visible spectroscopy, and scanning electron microscopy (SEM) are among the many methods used to thoroughly analyse the produced AC. According to the analysis of surface morphology, the AC has a large number of pores, which improves its ability to absorb organic pollutants. The efficacy of the produced AC in eliminating the organic dye Methylene Blue (MB) at a low concentration of 0.1 mg/mL is assessed. The outcomes show that, when it comes to MB concentrations of 1 mg/L, the AC demonstrates exceptional removal effectiveness. It's noteworthy that this high clearance efficiency is attained in a little over an hour. Both the Langmuir isotherm model and the pseudo-first-order kinetic model predict that MB will be adsorbed by AC. The Langmuir model highlights the possible use of AC in adsorption for the treatment of aqueous pollutants by indicating a maximum adsorption capacity for the material.

Keywords: Activated carbon, Methylene Blue, removal efficiency, Langmuir model.

Valorisation of Sand Hydrocyclone Washing Wastes (SHWW) as Flowable Fills for Sustainable Construction Practices

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Abstract

A circular economy envisages sustainable reuse of by-products and wastes, as opposed to the linear 'take-makeconsume-dispose' model. In order to meet the sustainable development goals (SDG) related to the construction sector, different strategies to produce sustainable construction materials using urban solid waste as secondary resources are of prime necessity. This study focuses on developing an innovative type of flowable fill known as Controlled Low Strength Material (CLSM), which is a self-compacting and low-strength mixture prepared primarily from Sand Hydrocyclone Washing Wastes (SHWW) obtained from granite quarries. The study evaluates both the fresh and hardened properties of the developed CLSM, including flowability, stiffening time, and strength performance. The laboratory results show that the designed CLSM at an optimal mixture ratio with fly ash and cement can provide 28-day compressive strength within the range of 0.7–1.12 MPa for a stiffening time of about 4 hours, and thus can meet the application requirements to produce prefabricated CLSM structures. Results from a pilot-scale implementation test proved the feasibility of the proposed CLSM to make contour bunds for erosion control in sloppy areas. This study demonstrates that SHWW can be potentially reused and successfully turned into a sustainable CLSM for large-scale field applications.

Keywords: Controlled Low Strength Material, Sand Hydrocyclone Washing Wastes, Flowability, Compressive Strength, Flowable fills.

Design Aspects of Lightweight Building Blocks using a Novel Mixture of Nanomaterials for Low-Cost Construction

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Abstract

Reducing the dead weight of structures is a major challenge in the construction industry in order to minimize shear damage in the foundations. The dead weight is primarily caused by the dead weight of the various building elements, which leads to high construction costs and susceptibility to risk. In order to minimize the self-weight of a structure without compromising the strength requirements, various lightweight materials can be used. The present study aims to investigate the suitability of three types of nanomaterials (lime - CaO, gypsum - CaSO₄.2H₂O and aluminum oxide - Al₂O₃) along with fly ash to develop building blocks. The experiments were conducted by casting concrete specimens by replacing the cement content (5-20%) sequentially in order to optimize the mixture proportions. Standard protocols were followed for casting and testing the specimens for their mechanical and environmental properties. The test results showed that an equi-molar mixture of lime, fly ash, gypsum and alumina exhibited higher compressive strength and durability compared to the other mixtures. The lightweight building blocks developed using nanomaterials are lighter, stronger and more durable compared to the alternative materials available. The selection of appropriate combination of nanoparticles is found to be critical in ensuring the desired engineering properties for the casted specimens. Further, the study advocates reuse of industrial wastes for preparing building elements thereby helping to achieve circular economy in the construction industry.

Keywords: Low cost building, Lightweight construction, Recycled nanomaterials, Optimized mixture proportioning.

A Comprehensive Structural Design-based Protocol for Energy-Efficient Buildings for **Smart City Projects**

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Abstract

As the global urban landscape continues to evolve, the need for providing sustainable and energy-efficient urban infrastructure becomes highly critical. For an existing urban settlement, the transformation to a smart city is constrained by lack of space and inefficient construction. Whereas, a developing city can adopt sustainability right from the design to the implementation by virtue of advanced materials and construction techniques. In addition to fulfill compliance with the standard criteria, further optimization becomes necessary to ensure safe and sustainable construction with energy and economic benefits. The present study proposes a comprehensive structural design-based protocol tailored for the construction of energy-efficient buildings within the context of smart city projects announced by Government of India. The framework addresses key parameters such as material selection, building orientation, passive design strategies, and innovative structural systems which includes structural analysis and design considering energy efficiency parameters such as renewable energy and ventilation space. By incorporating state-of-the-art technologies, such as sensor networks, building automation systems, and data analytics, the protocol aims to optimize the dynamic interplay between the structural integrity of the building with its energy performance. In order to reduce the carbon footprint and improve energy efficiency, building blocks made of recycled aggregates are suggested which can reduce the dead load and thermal insulation of the building. Ultimately, the study provides a valuable framework for the design of buildings in shaping the sustainability of urban spaces and aims to integrate advanced structural design principles into the fabric of smart cities.

Keywords: Smart city, Energy-efficient building, Sustainable construction materials, Structural design.

ICRTMD-2023/ST/293 Tuning the Structural and Dielectric Properties of ZnFe₂O₄ through Varied Annealing Temperatures

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Abstract

In this investigation, nano-crystalline ZnFe2O4 was synthesized via the sol-gel method, and we systematically examined the influence of annealing temperature on its physical characteristics. The average crystallite size, determined using the Debye-Scherres's formula based on Rietveld-refined X-ray diffraction data, exhibited a gradual increase from 16 nm to 58 nm as the annealing temperature elevated from 200 to 1000 K. Vibrational modes corresponding to metal-oxygen bonds at both octahedral and tetrahedral sites were evident in the FTIR spectra. UV-Vis DRS measurements revealed a discernible widening of the optical band gap from 2.03 eV to 2.14 eV with ascending annealing temperatures. The rearrangement of cations significantly impacted the dielectric properties and AC conductivity. Dielectric assessments illustrated a diminishing trend in both real and imaginary components of impedance with increasing frequency, decreasing from 107 at 100 Hz to 10 at 100 MHz. Furthermore, conductivity investigations underscored that the AC conductivity of $ZnFe_2O_4$ experiences enhancement at higher frequencies.

Keywords: Spinel Oxide; X-ray diffraction; Dielectric material;

ICRTMD-2023/ST/296 Investigation and Comparison of the Optoelectronic Properties of Natural Dyes Derived From Methanol and Aqueous Extract of Argyria cuneate Flower

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Abstract

In the preceding days, natural dyes derived from plant sources have become increasingly significant due to their easy-to-produce and biodegradable nature. Plants provide their colors so as not to harm the environment. There are hundreds of natural dye sources at our disposal. I have chosen Argyria cuneata, often known as Purple Morning Glory, as a common dye source for the present work. The current study focused on extracting natural colors from particular plant floral parts using aqueous and methanolic methods. Our methods for characterizing the extracted dye's optical characteristics included photoluminescence and UV-visible spectroscopy. This study involves the investigation of the colorant yield, molar absorption coefficient, refractive index, optical energy gap, and maximum emission range. The pigments found in flower extracts were examined using spectroscopic analysis, which produced energy band gaps and noticeable absorption peaks in the visible and UV regions. An authorized direct transition between the bonding and antibonding molecular energy states was to be the dye's optical absorption. The color achieved with methanol and water as the solvent yields the most emission. Because of this, the measurements observed here are essential to comprehending the material's suitability for UV and visible absorbers, optoelectronic devices, NDSSCs, and OLED applications.

Keywords: Argyria cuneate; Photoluminescence; UV-visible; refractive index; pigments.

Nano-Innovations in Post-Harvest Preservation: A Holistic Approach to Fruits and Vegetables

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Abstract

The global challenge of post-harvest losses in fruits and vegetables necessitates innovative strategies to enhance storage and preservation methods. This article explores recent advancements in the field, emphasizing the integration of nanotechnology and novel coating technologies to mitigate post-harvest losses effectively. This article also explores the synergistic effects of combining nanosensors for monitoring and nanoparticles for preservation within edible coatings, providing a holistic solution to address the multifaceted challenges associated with post-harvest management. By amalgamating diverse scientific disciplines, the paper highlights innovative solutions such as modified atmospheric storage, smart packaging and advanced preservation techniques to extend the shelf life of perishable produce. The purpose of this article is to offer a broad perspective on how packaging might be improved through incorporation of the natural active agents to develop smart and active packaging. As the world strives for sustainable agriculture and food security, this article underscores the importance of embracing cutting-edge technologies to minimize post-harvest losses. The integration of nanotechnology and innovative coatings not only enhances preservation efficacy but also aligns with the broader goal of promoting a more sustainable and resilient food supply chain.

Keywords: Post harvest losses; Active and Smart food packaging; Natural Polymers; Nanoparticles; Sustainability.

ICRTMD-2023/ST/301 Activation of charcoal at low temperature for electric double layer supercapacitor

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Abstract

Over the past few centuries, the history of humanity has been altered by the availability of energy. Our capacity to create and utilise energy has expanded with the emergence of new energy sources, including nuclear power, hydropower, fossil fuels, and now a range of renewable resources. Because of the advantages for the environment and the economy, scientists have concentrated on producing super capacitors (SCs) from a range of carbon sources, especially activated carbon (AC) from agricultural wastes. As a result, SCs have gained popularity as energy storage devices. Therefore, the goal of our work is to produce large surface area and electrochemically active charcoal ACs from oak wood charcoal. The quantity of activating agent used can alter the pore size and surface area of ACs. Characterizations of the materials show that micropores are created during activation and are utilised in the construction of the SC electrode. The electrochemical properties are monitored using the electrical impedance spectra, charging-discharging spectra, and cyclic voltammetry. The constructed AC-based SC exhibits good specific capacitance, power density, and energy density together with exceptional cycle stability.

Keywords: Activated carbon, electrode, supercapacitor, specific capacitance, power density, energy density.

ICRTMD-2023/ST/303 Natural Dyes To Light Harvesting Materials: A Study On Optoelectronic Properties Of Carissa Carandas Fruits

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Abstract

Natural dyes are being highlighted by research and industry trends; the majority of plant species offer abundant sources of colouring compounds. The intrinsic qualities of natural dyes include biodegradability, environment compatibility, lack of health risks, renewable nature, and ease of availability. They can be harvested using affordable technology and used in cutting-edge applications. Hence, an examination of the optoelectronic characteristics of Carissa caranda fruit dye has been looked into in this paper. Anthocyanins present in Carissa caranda were extracted by solvent extraction of the fruits with ethanol and methanol solvents, maintaining pH at 7 under room temperature. UV-visible spectroscopy analyzed the dye extracts, and the optoelectronic properties such as optical energy band gap, extinction coefficient, and refractive index, are studied. UV-Vis investigations revealed large absorption peaks in the visible area and obvious band gaps. Carissa caranda natural dye had the lowest direct bandgap of 2.98eV and an indirect bandgap of 1.93eV for ethanolic extraction. It was found that the optical absorption in the dyes obeyed both direct and indirect transitions between the molecular energy levels. FTIR spectroscopy has been used to confirm the composition of the natural dyes. The findings here may be particularly significant for organic electronics applications, including O-LEDs and sensors.

Keywords: Carissa caranda, Ethanol, Methanol, Optoelectronic parameters.

Drug kinetics and antimicrobial properties of quaternary bioactive glasses 81S(81SiO₂-(16-x)CaO-2P₂O₅-1Na₂O-xMgO); an in-vitro study

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Abstract

Bioactive glasses have recently been attracted to meet the challenge in bone tissue regeneration, repair, healing, dental implants, etc. Among the conventional bio-glasses, a novel quaternary mesoporous nano bio-glass with composition $81S(81SiO_2(16-x)CaO^2P_2O_5-1Na_2O-xMgO)$ (x = 0, 1.6, 2.4, 4 and 8 mol%) employing Stober's method has been explored for examining the above potential application through in-vitro SBF assay, MTT assay, antimicrobial activity and drug loading and release ability. With increasing the MgO concentration up to 4 mol%, from in-vitro SBF assay, we observe that HAp layer develops on the surface of the nBGs confirmed from XRD, FTIR and FESEM. MTT assay using MG-63 cells confirms the biocompatibility of the nBGs having high cell viability even after 168 h for 4 mol% of MgO (MGO 4). Moreover, MGO 4 has shown supreme antimicrobial properties against both E. coli and S. aureus. Despite an increase in magnesium concentration, nBGs are found to be non-toxic towards the RBCs up to 4 mol% of MgO. Being confirmed MGO_4 nBG as a bioactive material, various concentrations of drug (Dexamethasone (DEX)) loading and release kinetics are examined. We show that 80 % of drug loading and 70% of cumulative release in 100 h is observed in case of 10 mg-ml-1. The mesoporous structure of MGO_4 having an average pore diameter of 5 nm and surface area of 216 m2 g-1 confirmed from BET supports the loading and release kinetics. We conclude that the quaternary MGO_4 nBG may be employed effectively for bone tissue regeneration due to its high biocompatibility, excellent in-vitro cell viability, antimicrobial response and protracted drug release.

Keywords: Antimicrobial; Bioactive glass; Biocompatibility; Hydroxyapatite (HAp); Mesoporous; Protracted drug release.

Efficient Removal of Diclofenac Sodium using Cellulose-Based Luffa Actangula Peel Adsorbent: A Promising Approach for Water Treatment

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Abstract

Pharmaceutical Contaminants like NSAID are the rising concerns in the water stream affecting ecological system. An initiative is taken for removal of Diclofenac Sodium from the wastewater stream. A potential Luffa Actangula (Luffa A.) peel as a sustainable and low-cost adsorbent for the efficient elimination of DS is investigated in this study. Through a two-step procedure, a new cellulose-based adsorbent was synthesized from Luffa A. peels by alkaline treatment and bleaching method. Advanced analytical techniques such as Fouriertransform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), and Brunauer-Emmett-Teller (BET) analysis were used to characterize the prepared cellulose-based Luffa A. adsorbent. Various operating parameters were carried out such as pH, equilibrium time, concentration and temperature. The cellulose-derived Luffa peels (CLA) show excellent adsorption of Diclofenac sodium with a monolayer adsorption capacity of 153.54 mg/g within 60 minutes of equilibrium time at pH 3. The equilibrium data were well-represented by the Langmuir isotherm model, which proposed monolayer adsorption onto the adsorbent's plentiful cellulose moieties. The pseudo-second-order model, which is used in kinetic studies, best fits the experimental data and suggests that chemisorption is the predominant process. The evaluation of thermodynamic parameters, such as ΔH° , ΔS° , and ΔG° , verified that the adsorption process is endothermic. The CLA can be reused for upto five adsorption-desorption cycles by 0.1 mol L^{-1} acetone. Valorisation of easily available agricultural waste as a functional adsorbent provides a viable alternative for environmental cleanup while encouraging circular economy concepts.

Keywords: Diclofenac Sodium; Bleaching; Langmuir Isotherm; Desorption; Drugs.

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Abstract

In the present work, Mg doped ZnO thin film were synthesized on glass substrate by sol-gel spin coating method using Magnesium acetate tetrahydrate and Zinc acetate. And analyzed to observe the influence of the deposition variables such as constant heating temperature with different rotation speed. This is simple, economic and effective method to produce high quality films were structural, morphological and optical properties are studied. The structural properties of films were investigated by using X-Ray Diffraction (XRD), morphological studies were studied using Scanning Electron Microscopy (SEM), Energy dispersive X-Ray spectroscopy (EDS) and optical properties of films were studied by using UV-Visible Spectroscopy. XRD results showed that the films were polycrystalline nature and SEM and EDS images proved that the films were homogenous and compact. It was observed that the band gap increases as the rotation speed increases (3.13-3.37eV). The findings highlight the significance of controlled deposition variables in tailoring the characteristics of thin films for optoelectronic applications.

Keywords: MgZnO thin films, Sol-gel method, Spin coating method, Optoelectronic properties.

ICRTMD-2023/ST/317 Exploring the Impact of Strong Correlation and Spin-Orbit Coupling Effects in LuB₄: A First-Principles Study

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Abstract

Most of the rare-earth tetraborides, except YbB4, PrB4 show an anti-ferromagnetic ground state. In this work, we have investigated the electronic structure of LuB4, using first-principles density functional theory including the strong Coulomb correlation and spin-orbit coupling effects within GGA+U and GGA+U+SO approximations, as implemented in the VASP package. The ground state of LuB4 is determined to be non-magnetic due to the complete filling of 4f orbitals in the rare-earth atom. The projected density of states reveals three distinct spectral peaks well below the Fermi energy and separated from the continuum density of states around the Fermi energy. These discrete peaks arise due to Lu s, p and 4f orbitals respectively. Additionally, overlapping spectral peaks associated with B s and p orbitals appear between Lu p and 4f peaks. The continuum of states around the Fermi level arises due to hybridized B s, p and Lu d and 4f orbitals. Upon inclusion of SOC the spectral discrete peaks arising due to Lu p and 4f gets split into two peaks corresponding to j = 0.5, j = 1.5 and j = 2.5, j = 3.5 configurations, respectively. Inclusion of strong correlation effects leaves the qualitative features intact. However, notable shifts are observed in the positions of the Lu p and Lu 4f peaks toward and away from the Fermi level, respectively.

Keywords: Tetra-borides, DFT, Electronic strucure, Correlation effects, Spin-orbit coupling effect.

ICRTMD-2023/ST/318 Study of Surface Morphology & Elemental investigation of Chemically Deposited Mixed Based (Cdx-Pby-Znz)S Films

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Abstract

(Cd.x-Pby-Znz)S thin films have been deposited on glass substrates by cost-effective and very simple method called chemical bath deposition technique at 60°C in an aqueous ammonium solution of bath containing cadmium acetate, zinc acetate, lead acetate and thiourea using double distilled water at different concentration for their potential application in optoelectronic devices. X-ray diffraction (XRD) spectra revealed the structural properties of the films that deposited thin films exhibit both cubic and hexagonal crystal structure. Scanning electron microscope (SEM) Study for the Surface morphology of the as deposited films confirm that the cabbage type structure present in the sample and elemental study using Energy-dispersive X-ray analysis (EDAX) were done and it is confirm that all the elements used to prepared films are present. The Fourier transform infrared (FTIR) spectra show different chemical bonds present in the as-deposited film.

Keywords: Chemical bath deposition technique, X-ray diffractogram (XRD) spectra ,Scanning electron microscope (SEM), Energy-dispersive X-ray analysis (EDAX), Fourier transform infrared (FTIR).

ICRTMD-2023/ST/319 Study on the structural and electrical properties of Solid Oxide Fuel Cell (LaGaO₃)

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Abstract

The electrochemical devices known as solid oxide fuel cells (SOFCs) enable the direct conversion of fuels chemical energy into electrical power. Even though YSZ electrolyte–based conventional SOFCs are widely used in both laboratories and commercial scale, developing alternative ion conducting electrolytes in crucial to enhancing SOFC performance at lower operating temperatures. In this work, we conducted a through computational analysis of the characteristics of Sr- and Mg-doped a superior oxide ion conductor. We have used the DFT technique to examine the system electrical and structural characteristics as well as the impact of doping. The GII value and LaGaO₃, formational energy are used to investigate thermodynamical and structural stabilities, respectively. Theoretical practical are validated against data to ensure the accuracy of the computational model. On the research shows that the properties of Sr and Mg doped LaGaO₃ has changed in desirable way. This DFT study sheds light on the underlying mechanism affect the structural and electronic properties of LaGaO₃ electrolyte and offers a through investigation of the synergistic effects of strontium and magnesium co-doping. The knowledge acquired is critical to the logical design and development of more stable and efficient solid oxide fuel cell.

Keyword: SOFCs; Electrochemical devices; Electrolyte; DFT; Fuel cell.

Experimental and theoretical investigation into the effect of low energy C²⁺ ion irradiation on few layer WS₂

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Abstract

Material modification via ion beam irradiation is a controlled technique in the field of material science for processing nanostructures. These includes techniques, such as, ion implantation, ion beam mixing, particle irradiation, and focused ion beam (FIB) beams which are used to modify and manifest physical properties of a wide range of nanomaterials. In this work, our results highlight the introduction of carbon via low energy 15 keV C2+ ion implantation of tungsten carbide (WC) phase into tungsten disulfide (WS2) nanosheets. The coexistence of WC and WS2 hexagonal phases is suggested by X-ray diffraction (XRD) investigations at mid-fluences of ion implantation, which are typically in the range of $3.5 \times 10^{15} - 7.5 \times 10^{15}$ ions/cm². Additionally, the Raman peak position attributed to defects about 170 cm⁻¹ relates to the longitudinal acoustic (LA) mode at the M point of the Brillouin zone. Using first principles calculations, the geometric configurations and electronic structures of WS₂ were also examined both prior to and after implantation. Localised defect states were revealed in the conduction band (CB) of C-doped WS₂, with minima at the M point which corroborates to the LA(M) mode in Raman spectra. Notably, semi-metallic behaviour was observed, when C and S vacancies coexisted. The formation of an immiscible WC phase within a few-layered WS2 sheet is suggested to improve the material's strength and stability.

Keywords: 2D material; WS₂; implantation; Raman modes; DFT.

Thermal-Driven Formation of Reduced Graphene Oxide Nanosheets: A Novel Approach to Superior Supercapacitor Electrodes

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Abstract

In this investigation, thermally reduced graphene oxide nanosheets were synthesized through a thermal-assisted (hydrothermal) methodology by utilizing graphene oxide (GO) as the precursor material. GO was fabricated using the Tour method, followed by a thermal reduction process to yield rGO. A comprehensive array of analytical techniques, including X-ray diffraction (XRD), infrared spectroscopy, Ultraviolet-visible absorption spectroscopy (UV-Vis), and field-emission scanning electron microscopy (FE-SEM), were employed for material characterization. XRD analysis verified the crystalline nature of the synthesized rGO nanosheets. UV-Vis absorption spectro spectroscopy (FTIR). The surface morphology of rGO nanosheets was confirmed via field-emission scanning electron microscopy. An electrode was constructed on a graphite sheet utilizing rGO as the active material, and its electrochemical behaviour was systematically investigated employing cyclic voltammetry, galvanostatic charging-discharging, and electrochemical impedance spectroscopy within a 1M aqueous Na₂SO₄ electrolyte within a potential window of 0.8V. The electrodes demonstrated enhanced electrochemical performance, displaying a notable specific capacitance of 171 F g⁻¹ at a scan rate of 0.5 mV s⁻¹. The devised preparation protocol is considered by its simplicity, ease of implementation, environmental friendliness, and non-toxic nature.

Keywords: Reduce graphene oxide, Hydrothermal, XRD, Nanosheets, Supercapacitor.

Effect of Thickness on Structural, Morphological and Optical Properties of thermally evaporated Nichrome thin film

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Abstract

This paper provides the design, construction, and characterization of a neutral density filter (NDF) for the visible spectrum in order to improve color sorting applications. In this work, Nichrome single layer was designed by the Essential Macleod modelling software. The Co-evaporation of nickel and chromium was used to construct a filter on a glass substrate by thermal vacuum coating unit. Energy-Dispersive X-ray Spectroscopy (EDAX) examinations of the thin films revealed a constant stoichiometry for the chosen Nickel/Chromium ratio (80:20) during co-evaporation. Additionally, Atomic Force Microscopy (AFM) analysis revealed that surface roughness decreased from 6.034 to 2.895 in correlation with increased layer thickness. These methods made it possible to produce NDFs with optical densities ranging from 0.5 OD at an 11 nm film thickness to 2.7 OD at an 82 nm thickness. A good agreement was found between optical transmission and absorption spectra of the designed and the deposited films. The designed NDF's applicability and effectiveness for color sorting tasks were subsequently examined, marking a promising step towards advancing optical engineering solutions in this specific application domain.

Keywords: attenuator, optical coating, absorption, thin film, transmission.
Effect of Various Input Process Parameters on Surface Finishing and Materaial Removal Rate in Electrolytic Magnetic Abrasive Finishing

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Abstract

As per the demand of the industries for the machining of the matrerials with accuracy, there are so many options available in the market, hybrid machining is one of the method which is frequently used for the machining of the industrial component with accuracy. The Electrolytic Magnetic Abrasive Process is generally used as hybrid process in industries in which magnetic abrasive machining is combined with the electrolytic machining to get the better results compared with the individual one. Electrolytic magnetic abrasive finishing (EMAF) also saves the time and the hard materials are easily machined with this process. The machining parameters are having the major impact on the output results in any machining process. We can see the significant effect of the each parameter on output results by varying it and the range can be selected after prelimanary experimentation in which there is major improvement seen on the results parameters. The objective of this study is to investigate the workdone carried out by the different researched on the effects of the several input factors such as rotational speed of the work piece, machining time, concentration of the electrolytic liquid, electrolytic liquid flow rate, etc. on the output parameters of improvement in surface roughness and the removal rate of the workpiece (MRR) in EMAF process. The review of the study revealed that the rotational speed of the work materials and the electrolytic currents are the most significant parameters contributing in higher machining efficiency.

Keywords: Hybrid Machining, Electrochemical Machining, Material Removal Rate, Surface Finishing, Electrolytic Magnetic Abrasive Finishing.

Investigation of structural, electronic, and optical properties of Li doped hexagonal boron nitride monolayer through Green's function

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Abstract

As pristine hexagonal boron nitride (h-BN) exhibits a wide bandgap, its application in electronics, optical, and optoelectronic devices remain constrained, requiring structural modifications to overcome this challenge. This study delves into the investigation of the structural, electronic, and optical properties of a monolayer of h-BN doped with an alkali metal (Li), employing the quasiparticle-corrected Green's function (GW) method. The findings reveal the emergence of two defect states within the wide electronic bandgap of the h-BN monolayer, leading to a narrowing of the material's bandgap to 3.72 eV at the K- Γ point in the Brillouin Zone (BZ). The use of the GW approach over conventional DFT confers a distinct advantage, manifesting in qualitative shifts in band alignment. Furthermore, the presence of intra bandgaps, attributable to the two defect states, results in a redshift of the lowest excitonic peak from the deep UV region to the near-visible region at 1.61 eV. Consequently, Li doping in h-BN opens the door for the material's use in electronic, optical, and optoelectronic applications, effectively addressing the challenge posed by the wide bandgap in its pristine form.

Keywords: Boron-nitride; electronic properties; optical properties; doping.

Encapsulation of Bioactive Organosulfur Compounds in Solid Lipid Nanoparticles to Combat Multi Drug Resistance Pathogen

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Abstract

The escalating global challenge of combating pathogenic microbes requires innovative solutions to enhance the effectiveness of antimicrobial agents. Nanotechnology has emerged as a pivotal frontier, offering targeted and efficient drug delivery systems. This study introduces a cutting-edge approach to combat pathogenic microbes by utilizing solid lipid nanoparticles (SLNs) as carriers for potent antimicrobial compounds, specifically organosulfur compounds (OSCs) such as allyl sulfide (AS), diallyl disulfide (DADS), and diallyl trisulfide (DATS), known for their potent antimicrobial activity. Solid lipid nanoparticles are chosen for their biocompatibility, stability, and ability to encapsulate hydrophobic agents, making them an ideal platform for optimizing the therapeutic potential of antimicrobial compounds. In this study, the emulsification-solvent diffusion technique coupled with low-temperature solidification was used to encapsulate these OSCs into SLNs, resulting in a robust nanocarrier system designed for precise OSC delivery, controlled release, and improved bioavailability. This strategy effectively addresses key limitations associated with conventional antimicrobial treatments, including poor solubility, limited stability, bioavailability constraints, and potential side effects. Characterization of the OSC-SLN was performed using UV-VIS spectroscopy and FTIR, and loading capacity and encapsulation efficiency were also calculated. Antimicrobial activity was assessed against a multidrugresistant (MDR) strain of Bacillus cereus. The successful encapsulation of OSCs (AS and DADS) in SLNs was confirmed through UV spectrophotometric analysis and FTIR. The encapsulation efficiency and drug loading efficiency were determined to be as high as, 83.30±4.87% and 17.47±1.62% for AS-SLN and 79.15±3.67% and 15.78±2.52% for DADS-SLN, respectively. These OSC-SLNs exhibit significant antimicrobial activity against a variety of pathogenic microbes.

Keywords: Nanotechnology; Solid lipid nanoparticles (SLNs); Multidrug Resistance (MDR); Oragnosulphur Compounds (OSCs); Allyl sulphide (AS); Diallyl disulphide (DADS); Antimicrobial activity; Drug delivery.

Rheological, Physical, Thermal, Spectroscopical, Chemical and Electrical properties of novel organic draw solutes for forward osmosis desalination of brackish and seawater feed solutions

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Abstract

This study explored the use of novel binary organic draw solutions, combining a glycol ether (GE) with a cellulose derivative in forward osmosis (FO) processes. A total of 25 different mono or binary organic draw solution variants were prepared and analysed, leading to the selection of five solutions for further investigation. The osmotic pressures of the pure cellulose derivatives were compared with those of the binary solutions using a Freezing Point Depression Osmometer. The addition of GE to pure Hydroxylpropyl cellulose (HPC) draw solutions significantly increased osmolalities to levels necessary for FO desalination processes. The 0.5wt%, 1wt%, 1.5wt% and 2wt% pure HPC draw solutions had osmolalities of only 1, 8, 7 and 16 mOsm/kg respectively. Eleven of the initial organic draw solutions produced osmotic pressures greater than 25 bars. The thermal stabilities were determined using Thermogravimetric Analysis (TGA), for which the 2NaCMC-2NaCl comparison solution exhibited the highest thermal stability, enduring temperatures exceeding 500°C without complete degradation. The viscosities were determined using an Anton Paar MCR 302 Modular Compact Rheometer. The dynamic viscosities of the pure 1.5HPC, 1HPC, 2NaCMC, and 0.5HPC were reduced by 78.69%, 36.19%, 23.34%, and 11.6%, respectively, with the addition of an equal volume of 7.5M GE solution. The FTIR spectra of the combined 1NaCMC-7.5GE draw solution indicated that it was composed of a combination of the two individual solutions' wavenumbers. Furthermore, the study assessed the pH, electrical conductivity, and thermal profiles of the binary draw solutions. The refractive index of all the solutions decreased with an increase in temperature. The 1NaCMC-7.5GE was the most stable draw solution.

Keywords: Cellulose derivative, Forward osmosis, Osmolality, Desalination, Organic draw solution.

Preparation and Characterization of Self-Cleaning Hydrophobic Surfaces Using n(ZnO)Coated Glass

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Abstract

In the recent past, synthesis of metal oxide semiconductor nanoparticles has immensely attracted the attention of the researchers. Nanoparticles are widely used in solar energy production, catalysis, gas sensors, hydrophobic and scratchproof self-cleaning surfaces etc. Due to the substantial variations in their bandgap depending on their size and shape, zinc oxide nanoparticles find extensive use in various applications. Zinc oxide nanoparticles have a broad bandgap of approximately 3.3 eV. In this paper, we have reported preparation of n(ZnO) coated glass surfaces to introduce hydrophobic properties. We have prepared both spherical and nanorod like ZnO nanoparticles by green routes. We have used zinc acetate dihydrate [Zn(CH₃COO)₂·2H2O] and aqueous extract obtained from Dahlia Pinnata leaves. We obtain nearly spherical shape ZnO nanoparticles, when the pH values of the mixtures are maintained in the range of 6-8. The rod-like elongated nanostructures are obtained at pH 11. The unique morphologies of the n(ZnO) coated glass surface govern the self-cleaning properties. We use both experimental methods e.g. high-resolution X- Ray diffraction (HR-XRD), UV-vis-nir spectroscopy, Scanning Electron Microscopy (SEM) analysis, Fourier Transform Infrared Microscopy (FTIR), Optical Microscopy (OM) etc. and DFT based theoretical methods to investigate the bandgap values of ZnO nanoparticles as well the self-cleaning properties of the surfaces.

Keyword: Self-cleaning; Dahelia Pinnata; SEM, FTIR, HR-XRD, UV-vis-nir; Optical Microscopy; High resolution.

Green Synthesis of Magnesium Oxide NPs Using Chea Seeds and Investigation of Their Antibacterial Effect

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Abstract

The fascination towards using green synthesis methods is growing fast and acquiring the attention of researchers seeking safer and biocompatible processes for nanoparticle production. Green synthesis methods have gained prevalence in industries over customary physicochemical approaches. This study delves into an environmentally conscious approach for the synthesis of magnesium oxide (MgO) nanoparticles, employing a seed extract derived from Salvia Hispanica also commonly refered as chia seed, with a primary focus on assessing their antibacterial potential. This not only reduces the environmental impact associated with traditional methods but also guarantees the generation of NPs with improved biocompatibility. The usual methods include extracting bioactive compounds from seeds, which function as efficient reducing agents, initiating the reduction of magnesium salts and leading to the creation of MgO NPs. The seed extract not only facilitates the nucleation and growth of nanoparticles but also impacts the distinctive properties of the resulting MgO NPs. The synthesis includes extracting active components from plant sources to serve as reducers and transforming magnesium precursors into crystalline MgO NPs. Characterization via high-resolution X-ray diffraction (HR-XRD). Fourier-Transform Infrared Spectroscopy (FTIR) and Scanning Electron Microscopy (SEM), confirm the successful production of NPs with controlled size and morphology. The antibacterial capabilities of MgO NPs were evaluated against various bacterial strains using PCR technique. This investigation provides valuable insights into the antibacterial attributes of MgO NPs, paving the way for further exploration of their potential in combating bacterial infections. We also compare the antibacterial properties of MgO NPs with ZnO NP samples prepared using zinc acetate dihydrate [Zn(CH₃COO)₂·2H₂O] and aqueous extract obtained from Dahlia Pinnata leaves.

Keywords: MgO NPs, ZnO NPs, Salvia Hispanica, Dahlia Pinnata, Antibacterial effect, Specific Surface Area, Physio-chemio-sorption.

ICRTMD-2023/ST/335 Tailoring optoelectronic properties of hydrothermally synthesized Sn-doped nickel oxide thin films

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Abstract

This study investigates the synthesis and characterization of tin (Sn) doped nickel oxide (NiO) thin films tailored for optoelectronic applications. Sn-doped samples were prepared via a hydrothermal method, varying Sn concentrations from 0% to 10%. The characterization involved X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), UV-Visible spectroscopy (UV), Fourier transform infrared spectroscopy (FTIR), and electrical analysis. XRD analysis validated the cubic phase and confirmed the structural integrity of the synthesized samples. FESEM elucidated surface morphology, revealing variations in nanoparticle size and shape with differing Sn concentrations. Utilizing Tauc's plots, direct optical band gaps of the samples were determined, ranging between 2.90 and 3.30 eV. The increase in Sn doping concentration exhibited a proportional enhancement in IV characteristics, indicating improved electrical properties. Remarkably, photocurrent spectra showcased a substantial augmentation in current as Sn doping increased, underscoring the enhanced optoelectronic properties. The findings suggest the potential for tailored control over morphological and optical characteristics of Sn-doped NiO through the straightforward hydrothermal method employed in this study. These outcomes establish the viability of Sn-doped NiO thin films for diverse optoelectronic applications, offering promise for advanced device functionalities in the field.

Keywords: Sn-doped nickel oxide; Hydrothermal method; Optoelectronic properties; I-V characteristics.

Synthesis of Nano-crystalline Thin Ferromagnetic Films and Investigation of Their Thickness Dependent Magnetic Properties

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Abstract

The systematic examination of multiple phases in iron oxide nanostructures highlights their inherent importance, with the goal of understanding their magnetic behavior which depends upon these phases. This research article delves into the effects of annealing the thin films formed by iron oxide nanoparticles kept at 200, 300 and 400 °C for different durations. We first synthesize iron-oxide nanoparticles using chemical co-precipitation method by adding ferric nitrate into de-ionized water (0.2 M). Ammonium hydroxide is used to maintain the pH of the solution. 0.2 M SDS was used as a capping agent. We prepare films of different thickness composed of iron-oxide nanoparticles on glass substrates via spin coating method. Increasing the annealing time under an oxygen flow increases the volume fraction of α -Fe2O3 and improves the crystalline nature of the Fe3O4 phase, as reflected in magnetization patterns over time. An optimal annealing duration for a given temperature maximizes the concurrent presence of both phases, resulting in increased magnetization and an interfacial pinning effect. This effect is attributed to the disordered spins that separate magnetically distinct phases, aligning under the influence of a magnetic field at elevated temperatures. The magnetic properties of the film also depend on the size and shapes of the iron-oxide nanoparticles, which can be controlled.

Keywords: Annealing effect, Nano-crystalline, Spin Coating, BH curve, Pinning effect.

Synthesis of silver Nanoparticles used in tridax procumbens leaf extract and their characterization

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Abstract

Plant-mediated synthesis of nanomaterials has been increasingly gaining popularity due to its eco-friendly nature and cost-effectiveness. In the present study, we synthesized silver (Ag) nanoparticles using aqueous extracts of fresh leaves tridax procumbens and medicinal plants as bio reducing agents. This method allowed the synthesis of nanoparticles, which was confirmed by ultraviolet-visible (UV-Vis) spectrophotometry and transmission electron microscopy (TEM). UV-Vis spectra and visual observation showed that the color of the fresh leaf extracts of tridax procumbens turned into grayish brown and brownish yellow, respectively, after treatment with Ag precursors. In addition, TEM analysis confirmed that AgNO3 solutions for all concentrations produced Ag nanoparticles and their average size was less than 24 nm. Moreover, aqueous leaf extracts of tridax procumbens were separately tested for their antimicrobial activity.

Keywords: Nanomaterial, Tridax procumbens extract.

Synthesis of Carbon Nanodots via Green Routes and Investigation of Their Antiviral Effect

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Abstract

This inquiry resulted into the production of carbon nanodots through an eco-friendly and cost-efficient sol-gel preparation technique. This research work highlights the antibacterial efficacy of carbon nanodots prepared via green routes using plant leaves, roots and their stems. The paper unveils the underline mechanisms dictating the antibacterial and antiviral effectiveness of carbon dots. Through a series of experiments, we showcase the robust antibacterial capabilities of carbonnanodots across diverse bacterial strains. Stable carbon nanodots were prepared from neem and aloevera leaves and characterized by UV-vis-nir spectroscopy, fluorescent spectroscopy, Fourier Transform Infrared (FTIR) spectroscopy, Scanning Electron Microsciopy (SEM), Dynamic Scattering Light and Raman's spectroscopy techniques. The different antibacterial applications of C-dots such as antimicrobial activity against staphylococcus aureus, Ecoli, chikungunya virus etc have been explored. We have synthesized the C-dots from neem leaves and aloevera extract. Both shows antibacterial effect though C-dots prepared using neem extracts are found to be better for external uses. This research reveals that C-dots synthesized from neem leaves and aloevera are useful therapeutic agents to fight against human microbial infections.

Keywords: Carbon nanodots, Neem, Aloevera, Green synthesis, Antibacterial effect.

M^{II}[Zn/Mg/Ni]Al-NO₃/Cl Layered Double Hydroxide as Electrode Material for Dye **Sensitized Solar Cell Application**

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Abstract

Layered double hydroxides (LDH) belong to the class of anionic clay layered materials and have been extensively evaluated in the field of energy production and storage on account of their physiochemical, thermochemical, mechanochemical and electronic properties. In this study, LDHs have been evaluated as the component material in dye-sensitized solar cells (DSSC). The photovoltaic application of chloride and nitrate intercalated M^{II} [Zn/Ni/Mg] Al- LDH with molar ratio (3:1) as the working electrode for dye-sensitized solar cell has been studied using beetroot natural dye with KI and I2 as electrolyte and ITO/FTO glass slides. The performance and efficiency of LDH material in both cases as photoanode and counter electrode in terms of open circuit voltage (Voc), short circuit density (Jsc) and fill factor (FF) were measured.

Keywords: Layered double hydroxide, Dye-sensitized solar cell, Counter electrode, beetroot, photoelectrode.

Green Synthesis And Characterization Of Cow Dung/Bamboo Fibre Derived **Polyaniline-Based Composite for Energy Application**

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Abstract

Polyaniline (PANI) is considered a conducting polymer and has various physical and chemical properties. It is used in multiple applications such as biosensors, biomedical fields, and electronic devices. Cow dung is one of the most abundantly available rural resources. It is pre-digested in cattle's abdomen and hosts various microorganisms facilitating soil conditioning, pest repellency, and pathogen management. Conventionally, cow dung has been used extensively in organic and commercial agriculture. Bamboo is one of the most treasured natural resources available with abundant of cellulose in it. The present work reports the Green Synthesis of different composites Cow Dung/Bamboo Fiber fiber-derived polyaniline-based Composite by the chemical route using microwave and ultrasonication techniques. The developed samples were characterized for various properties such as physiochemical properties, electrical impedance,FTIR, microscopic etc. The developed Cow Dung/Bamboo Fiber Derived Polyaniline-Based Composite are useful for a broad application spectrum. The work proposes one of the appropriate uses for the large volume of cow dung and bamboo fiber produced globally.

Keywords: Cow Dung; Bamboo Fiber ;Microwave;Polyaniline; Composite.

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Investigating the Thermal and Mechanical Synergy of PEEK/GNP Nanocomposites

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Abstract

In this study, we delve into the thermal and mechanical characteristics of PEEK/graphene nanoparticle nanocomposites, serving as a model to unravel the intricate interplay between nanoparticles and polymers. Our aim extends to uncovering potential engineering applications for these nanocomposites. The choice of Poly (ether ether ketone) (PEEK) stems from its impressive chemical resistance, outstanding mechanical traits, and elevated thermo-oxidative stability. Meanwhile, graphene nanoparticle (GNP) is selected for its distinctive features-high optical transparency, superior heat conductivity at room temperature, and flexibility encapsulated within a robust nano-sized material. Our research is centered on crafting PEEK/GNP polymer composites with varying GNP concentrations through the utilization of a co-rotating twin-screw extruder. Thorough characterization employing diverse analytical techniques such as Fourier transform infrared spectroscopy (FTIR), differential scanning calorimetry (DSC), and thermogravimetric analysis (TGA) accompanies the fabrication process. Mechanical property evaluations are conducted using a universal testing machine (UTM), impact tester, and hardness tester. Our findings underscore the substantial advantages of GNP incorporation, fostering enhanced interfacial adhesion and establishing favorable interactions between PEEK and GNP. Notably, the addition of GNP elevates the ductility and toughness of the PEEK/GNP composites. This study culminates in the revelation that the PEEK/GNP composite with a 0.3% concentration of GNP (PG3) showcases remarkable thermo-mechanical properties.

Keywords: PEEK; GNP; Thermal Properties, Mechanical Properties, Characterization.

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Robust Synthesis and Antimicrobial Applications of Bismuth Oxide/ Graphene Oxide Derived Poly(Vinyl Alcohol) based Nanocomposite as Biomedical Material

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Abstract

The present study focuses on the synthesis and antimicrobial applications of Bismuth Oxide/ Graphene Oxide Derived Poly Vinyl Alcohol based Nanocomposite as Biomedical Material. The sample was prepared using bismuth nitrate as a precursor and Cytosine as Capping agent by a novel chemical route using an ultrasonicator. The synthesis process of incorporating citric acid to crosslink PVA establishes a stable gel and glycerol chemically to develop the Bismuth Oxide/ Graphene Oxide Derived Poly Vinyl Alcohol based Nanocomposite. The samples were developed with various percentages of Graphene Oxide incorporated in them and were characterized using sophisticated techniques such as physiochemical properties, Surface morphology, and antimicrobial properties. The antibacterial, anti-fungal and anti viral effectiveness was evaluated against gram-positive Staphylococcus aureus and gram-negative bacteria E.coli, demonstrating the potential of developed material for diverse antimicrobial characteristics, notably in biomedical fields. The MIC studies, antioxidant characteristics etc. were also performed in the developed sample. The outcomes suggest promising prospects for utilizing this gel as an efficient strategy against bacterial infections in the biomedical sector.

Keywords: Polyvinyl Alcohol; Bismuth Oxide; Graphene Oxide; Antibacterial

Size Dependent Estimation of Bandgaps: From Synthesis to Formulation

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Abstract

The estimation of bandgaps in nano-structured materials is a crucial aspect of understanding their electronic properties. It also helps to explore their potential applications in various fields by bandgap engineering via controlling their shapes and sizes. Owing to their confinement in size and shape, nano-sized materials, exhibit distinct electronic configurations that deviate from their bulk counterparts. The bandgap, which represents the energy difference between the valence band and the conduction band, plays a pivotal role in determining the material's optical, electrical and electronic properties. Quantum confinement effects become prominent as the size of a material approaches the nanoscale. The bandgap can be estimated using models like the effective mass approximation or tight-binding models, taking into account the size and shape of the nanostructures. We have synthesized different nanomaterials e.g. ZnO, MgO, ZnS, CdS, CuO and Fe3O4 etc using sol-gel and chemical co-precipitation methods. We evaluate their bandgaps using edge wavelengths obtained from UV-vis-nir data as well as from Tauc plots. We also perform quantum mechanical stimulations, such as density function theory (DFT) calculations to obtain the bandgaps of some of the nanomaterials to explore the underline science. These computational methods consider factors like atomic arrangement, size, and surface effects to accurately estimate electronic properties. The comparison between the experimentally determined bandgap values and those obtained and predicted from theoretical models based on nanoscale principle are then compared to explore the size and structure dependent bandgap values.

Keywords: Band-gap-engineering, UV-vis-nir, Tauc plot, SEM, HR-XRD, FTIR.

Synthesis And Study Of Thermal Insulating Characteristics Of Bio Sludge / Fly Ash-Based Geopolymer Binder Composite Material For a Sustainable And Constructive Approach

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Abstract

This study intended to ascertain the most effective way to Synthesis And Study the Thermal Insulating Characteristics Of Bio Sludge / Fly Ash-Based Geopolymer Binder Composite Material For a Sustainable And Constructive Approach. The work supports the environmental challenges: fly ash - a specific waste from the thermal power plants, and bio sludge from the local fish pond. This study combined various ratios of fly ash and bio sludge and created composite material in the form of tiles for environmentally friendly construction approaches. The sample is studied for various characterizations such as physicochemical, Mechanical, thermal conductive, XRD, SEM etc. The results validate the use of Fly ash, and bio sludge as materials for sustainable development. The study's findings demonstrate that fly ash waste powder may effectively stabilize bio sludge, producing a stable composite material. This type of waste management offers an ideal zero-waste solution from the perspective of sustainable development since it produces cleaner output while protecting natural resources, cutting CO_2 emissions, and lowering biosludge and fly ash management expenses. The developed sample can be used for a broad application spectrum such as construction sector.

Keywords: Bio sludge; Fly ash; Sustainable.

Photocatalytic Reaction Chemistry of Sustainable Graphene Aerogel for Sequestration of Pharmaceutical Residues

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Abstract

A sustainable graphene aerogel has been synthesized and sugar was used as a precursor. The aerogel consists of heteroatoms i.e., O, and N confirmed by XPS. The presence of heteroatoms perturbed the electrical neutrality of the framework leading to enhance physicochemical properties. A good interconnected framework revealed by FESEM has encouraged us to investigate the photocatalytic activity of the material. Aerogels are the potential candidate for such applications as they are easy to recover without any chemical treatment with high activity. Pharmaceutical waste is one of the water pollutants, so in this research, Telmisartan (Tel) was chosen as pharma waste used to treat high blood pressure. The synthesized graphene aerogel has shown high photocatalytic activity for the degradation of Tel solution within 70 min with 90% of recyclability. The driving force for the ease of formation of radicals or reactive oxygen species (ROS) is governed by heteroatoms and herein, the superoxide is a major ROS for photocatalytic activity.

Keywords: Photocatalysis, graphene, aerogel, heteroatoms, biomass, reactive oxygen species.

Study of Effort of Temperature and Binder on Brine Sludge Based Composite Material

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Abstract

Innovative waste management solutions are particularly needed in companies that generate a lot of byproducts, because of the increasing problems related to environmental sustainability. Desalination is an industry that involves extracting freshwater from saltwater sources, resulting in the production of brine sludge. Despite its mineral richness, this waste product is problematic for the environment because of the need to dispose of it. This study sets out to investigate the feasibility of using brine sludge as a component in the production of composite materials. By incorporating brine sludge into composite matrices, a viable solution is found for its disposal, transforming it into a valuable resource instead of simply discarding it. However, the effectiveness of such composites relies on a range of factors, including the temperature conditions during synthesis and the choice of binder. A sequence of carefully planned experiments were undertaken in order to clarify the complex interconnections among these variables. The study methodically manipulated the temperature parameters to simulate a wide range of climatic conditions. It also included a variety of binders to investigate both their combined and individual impacts on the properties of the composite material. The findings revealed thoughtprovoking observations. The composite materials' mechanical strength, thermal stability, and structural integrity were significantly impacted by both temperature fluctuations and the selection of adhesive. Some binder formulations demonstrated better performance results within specified temperature ranges, suggesting possible ways for optimising them for specific applications. In the end, this study not only shows that it is possible to turn brine sludge into materials with added value, but it also gives us a better understanding of how processing factors affect the properties of the materials. These ideas are very important for making the desalination industry more sustainable, promoting smart waste management, and supporting the growth of composite materials that are good for the environment.

Keywords: Brine sludge, composite material, environmental sustainability, optimization.

ICRTMD-2023/ST/367 Innovative Approach to Achieving Zero Liquid Discharge in the Dye Intermediate Sector

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Abstract

The dye intermediates industry plays a pivotal role in the textile, paper, and chemical sectors, but it is often associated with significant water pollution due to the release of complex and colored effluents. Consequently, there are serious environmental and health risks associated with the untreated, continual outflow of wastewater from several dye factories. There is concern that dyes, which pollute aquatic ecosystems, may be harmful to aquatic creatures and even make it into human diets. This paper explores the implementation of Zero Liquid Discharge (ZLD) as a sustainable solution to address the environmental challenges posed by the dye intermediate industry. The paper delves into the specific challenges faced by the dye intermediate industry, such as the presence of recalcitrant organic compounds and intense coloration in wastewater. It examines how ZLD systems, which typically involves highly energy demanding and costly treatment methods can be replaced by comparatively cheaper methods which can be afforded by small scale industries to achieve environmental compliance and resource conservation. The paper explores and evaluates the framework of ZLD based on several criteria which includes prevention of water pollution, the preservation of water resources, compliance with stringent environmental regulations, economic and operational advantages. The economic and operational advantages of ZLD are also highlighted.

Keywords: Zero Liquid Discharge, Dye Intermediate, Water Pollution, Resource Conservation.

A Neural Network Approach to Enhance FDM 3D Printing Parameters for PETG: Optimizing Compressive Strength and Surface Roughness with Validation Using MOGA-ANN

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Abstract

The mechanical properties of 3D-printed components are intricately influenced by the interplay of fused deposition modeling (FDM) process parameters and material properties. The experimental investigation focuses on analyzing the distinct influence of the most significant process parameters, namely layer height, infill density, and shell thickness, on both the compressive strength and surface roughness of Polyethylene Terephthalate Glycol (PETG). Specimens are manufactured as per ASTM standards, incorporating various combinations obtained from the systematic design of experiments (DOE) of the aforementioned process parameters. The maximum compressive strength achieved is 47 MPa, characterized by a layer height of 0.2 mm, infill density of 80%, and Shell thickness of 0.8 mm. Simultaneously, the lowest mean surface roughness (Ra) recorded is 3.42 μ m realized at a layer height of 0.1 mm, infill density of 60%, and Shell thickness of 0.8 mm. To refine and validate these results, artificial neural network (ANN) optimization techniques are employed, followed by validation through a multi-objective optimization approach using a genetic algorithm (MOGA-ANN).

Keywords: 3D printing; Fused deposition modelling; Process parameter; MOGA-ANN; Genetic Algorithm.

Nano Wear Circuits: Multiwalled Carbon Nanotubes Transforming Yarn into Strain Sensors

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Abstract

The continuous monitoring of various parameters has led to the widespread use of wearable sensors, with smart yarns and textiles being a particularly active area of research due to their potential applications in wearable devices and electronic sensors. By incorporating conductive fillers into ordinary yarns, composite yarns with new and intriguing functions can be created, such as the ability to sense and monitor strain and stress. In this study, a wearable strain sensor was fabricated using multiwall carbon nanotubes (MWCNTs) synthesized through the Chemical Vapor Deposition (CVD) method. The optical, structural, and tensile strength properties of the MWCNTs were characterized. These MWCNTs were then coated onto several types of yarns, including nylon, polyester, silk, and cotton, using a dipping method. Silver contacts were added to the yarns to measure the strain parameters. The impedance characteristics, piezo-resistive properties, repeatability, and gauge factor of the strain sensors were investigated by applying different loads. Among all the yarns, nylon yarn exhibited excellent sensitivity and strain variation, particularly in terms of its specific piezo-resistive property.

Keywords: Multiwall carbon nanotubes, Wearable strain sensor, Yarn breaking strength.

ICRTMD-2023/ST/381 In today's High-Frequency Environments, Heterostructured 2D MoS₂/Ferrite Nanocomposites Serve as Exceptional Microwave Absorber Material

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Abstract

The modern world places a high priority on addressing electromagnetic pollution and developing sustainable materials for stealth applications. Significant efforts are being made to develop advanced microwave absorption materials (MAMs), with an emphasis on environmentally friendly solutions. As a contribution to recent research, a novel approach to creating single-layer microwave absorbers using metal sulfide/Ferrite by hydrothermal method has been introduced. These absorbers have exceptional properties because they are made of 2D MoS2/Ferrite nanocomposites (MSF). They are remarkably thin and lightweight, with a thickness of only 1.5 mm, and when combined with paraffin wax, they achieve a weight-to-weight ratio of 1:1. Furthermore, these materials are intended to perform well in the high-frequency range of 26 - 40 GHz, also known as the Ka-band. This frequency range is also crucial in 5G communication technology. A 2D heterostructure's larger surface area with multiple interfaces that influences the substance's ability to absorb microwaves. As a result, it absorbs microwaves more efficiently. The results show that the material achieves a reflection loss value of - 32.83 dB at 26.07 GHz with a thickness of 1.5 mm, indicating a high attenuation constant and an absorption rate of 99.999%. The exceptional performance of this material suggests that it could be used in the development of military applications, anechoic chambers, and cost-effective textile industry stealth materials. It is worth noting that these results outperform many other metallic sulfide and metallic oxide materials and their nanocomposite materials previously reported using various synthesis methods and structures.

Keywords: 2D-MoS2/Ferrite(MSF), Hydrothermal Method, High Frequency, 5G Communication Technology, Microwave Absorption.