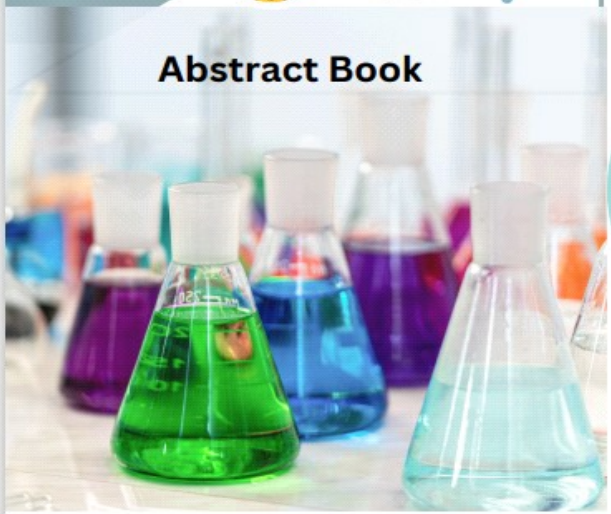
4th International Conference
On
Recent Advances in Interdisciplinary Sciences

4-6 December-2024

ICRAIS-2024

Abstract Book



Chief Organizer
Dr. Abida Kausar
Chairperson
Department of Chemistry
GC WOMEN UNIVERSITY FAISALABAD

Thematic Areas

1. Nano-chemistry & Nanotechnology Applications
2. Emerging Technologies in Environmental Sciences
3. Frontiers in Nutrition /Food Chemistry
4. Interdisciplinary Research Trends
5. Natural & Synthetic Medicinal / Pharmaceutical Sciences by Integrated Computational Approach
6. Smart & Sustainable Development in Materials Manufacturing & Energy

Program Highlights

- Keynote & Plenary Talks
- Video Presentations
- Poster Presentations
- Oral Presentations
- Hands on Training on Data Analysis

For Submission of Abstracts and Poster Presentations Contact to
Dr. Farhat Jubeen
conference@gcwuf.edu.pk

Poster Competition 2024

Registeration Fee for
Faculty; 4000/-
Students; 2500/-

Link for Registration
https://profile.gcwuf.edu.pk/CHEM/

Conference Scope

The scope of conference is to bring together a unique and world-class blends of professionals from across the globe, encompassing researchers, scientists, analysts, and leaders from both the research community and industry. The conference aims to facilitate the exchange of insights, experiences, and research advancements in the field of Natural Sciences, providing a comprehensive platform for interdisciplinary collaboration and knowledge dissemination.

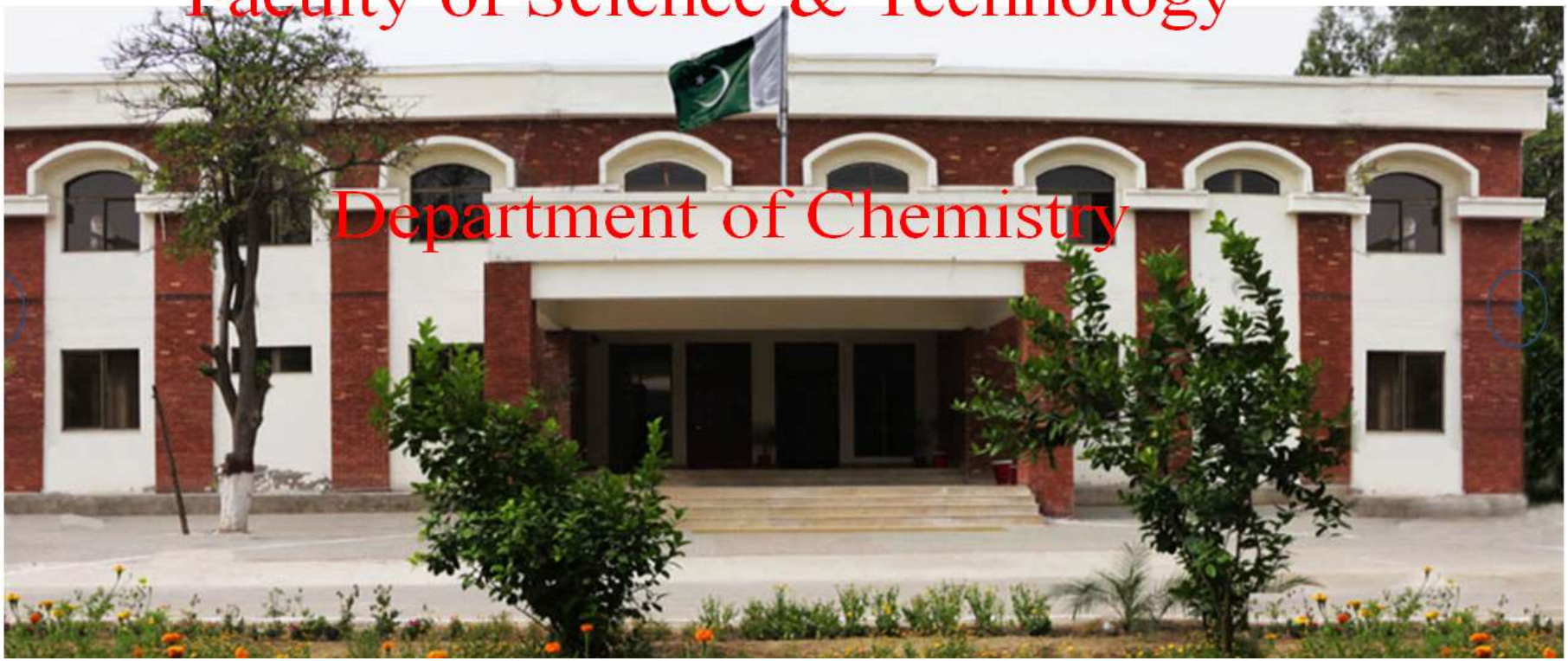
Objectives

- To Promote Interdisciplinary Collaboration
- Exchange of Cutting-edge Research
- To Address Practical Challenges
- To Encourage Knowledge Sharing

Professor Dr. Kanwal Ameen
Tamgha e Imtiaz (T.I.)
Patron-In- Chief
Vice Chancellor GC Women University Faisalabad

Government College Women University Faisalabad

Faculty of Science & Technology



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Vice Chancellor
Government College Women University Faisalabad

Patron

Prof. Dr. Zill-i-Huma Nazli
Pro-VC
Co-ordinator Science & Technology
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Associate Professor
Department of Chemistry
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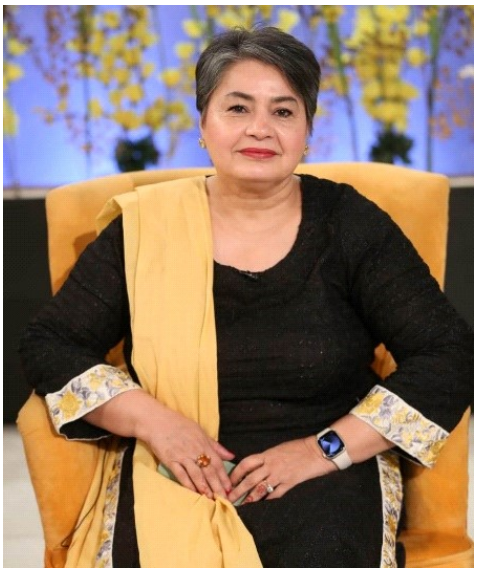
Welcome Note by Prof. Dr. Kanwal Ameen (T.I)

Vice Chancellor (Patron-in-Chief)



Assalamu Alaikum and a very good morning to all of you. It is with immense pleasure and pride that I welcome you to 3 Day International Conference on Recent Advances in Interdisciplinary Sciences. As the Vice Chancellor of Govt College Women University, Faisalabad, it is my honor to inaugurate this prestigious event. This conference is a testament to our commitment to fostering innovation and collaboration across various scientific disciplines. In today's rapidly evolving world, the integration of knowledge from different fields is not just beneficial but essential for addressing complex global challenges. Over the next three days, we will witness a confluence of ideas, where experts from diverse domains will share their insights and discoveries. Moreover, this conference provides an invaluable opportunity for networking and professional growth. Participants will have the chance to connect with leading experts, engage in thought-provoking discussions, and explore potential collaborations that can extend beyond the duration of the event. I can see a number of eminent speakers from various fields of sciences, looking enthusiastic to share their endeavors. I am confident that this conference will serve as a platform for fruitful discussions, inspiring new research directions and forging lasting partnerships. The exchange of knowledge and experiences here will undoubtedly contribute to the advancement of science and technology, benefiting society at large. I am pretty much confident that you will witness excellent hospitality from Manchester of Pakistan, this year here in GCWUF.

Welcome Note by Prof. Dr. Zill –i- Huma Nazli

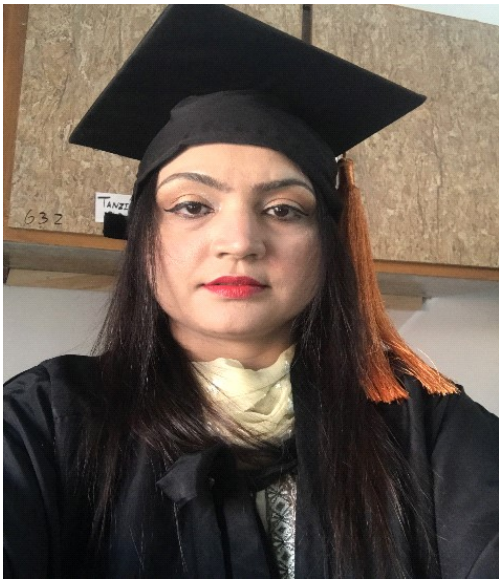
Pro-Vice Chancellor (Patron)

Distinguished Guests, Esteemed Colleagues, Respected Scholars, and Dear Students, Assalamu Alaikum and a very warm welcome to each one of you. It is my great pleasure to extend my heartfelt greetings as we gather for the International Conference on Recent Advances in Interdisciplinary Sciences. As the Pro Vice Chancellor, I am honored to be part of this significant event. This conference is a proof of our collective commitment to advancing scientific knowledge through interdisciplinary collaboration. In today's world, the challenges we face are complex and multifaceted, requiring innovative solutions that transcend traditional boundaries. By bringing together experts from diverse fields, we create a unique platform for the exchange of ideas, fostering a spirit of collaboration that is essential for groundbreaking discoveries. The importance of this conference cannot be overstated. It provides an invaluable opportunity for researchers, scholars, and practitioners to share their latest findings, discuss emerging trends, and explore new methodologies. The interdisciplinary approach not only enriches our understanding but also opens up new avenues for research and application, ultimately benefiting society as a whole. Moreover, this conference serves as a catalyst for professional growth and networking. It allows participants to connect with leading experts, engage in meaningful discussions, and forge partnerships that can lead to future collaborations. The knowledge and connections gained here will undoubtedly have a lasting impact on our respective fields and beyond. I am confident that the insights and innovations shared during this conference will contribute significantly to the advancement of science and technology. Let us embrace this opportunity to learn from each other, inspire one another, and work together towards a brighter future. Thank you for being here and for your active participation. I wish you all a successful and enriching conference.

Welcome Note by Dr. Abida Kausar

Chairperson, Department of chemistry, GCWUF

(Convener)



A very Good morning in Faisalabad, Distinguished Guests, Esteemed researchers, and dear students, It is with great pleasure and honor that I welcome you to three day international conference "Recent Advances in Interdisciplinary Natural Sciences (RAINS)." From the integration of physics and biology, chemistry, data science, and environmental studies to address global challenges, interdisciplinary approaches are not just desirable—they are imperative.

Today, we are privileged to have a remarkable assembly of thought leaders, researchers and young learners in this event to provides a valuable platform to exchange ideas, ask questions, and spark new collaborations that could shape the future of natural sciences. I encourage each of you to actively participate in the sessions, engage in meaningful discussions, and take advantage of the opportunity to network with like-minded peers. We are delighted to host an extraordinary lineup of keynote speakers, panel discussions, and presentations covering topics that are shaping the future of science and technology. Your active participation and contributions will undoubtedly make this event a success and pave the way for meaningful advancements in our field.

Before we proceed, I would like to extend my heartfelt gratitude to the organizing committee, sponsors, and participants who have worked diligently to bring this event to life. Your efforts and dedication have been instrumental in making this conference a reality.

Once again, welcome to the conference on "Recent Advances in Interdisciplinary Natural Sciences." Let us use this occasion to inspire, learn, and contribute to the advancement of knowledge that benefits both science and society.

Guests of Honour, Keynote & Invited Speakers, International Speakers & National Speakers

Welcome

4th International Conference on "Recent Advances in Interdisciplinary Sciences"

Patron -in- Chief
Prof. Dr. Kanwal Ameen
Tamgah-e-Imtiaz (T.I.)
Vice Chancellor GC Women
University Faisalabad

Patron
Prof. Dr. Zill-i-Huma Nazli
Pro-Vice Chancellor GC Women
University Faisalabad

Plenary Speakers

Prof. Dr. Shazia Anjum, Vice Chancellor, The Government Sadiq College Women University Bahawalpur - Pakistan

International Speakers

Prof. Mark Moloney, Emeritus Depat. of Chemistry, University of Oxford, UK

Prof. Dr. Halil İbrahim Ulusoy Analytical Chemistry Department, Faculty of Pharmacy, Sivas Cumhuriyet University, SIVAS/TURKİYE

Invited Speakers

Prof. Dr. Muhammad Akhyar Farrukh Dean , Faculty of Science and Technology, University of Central Punjab, Lahore

Prof. Dr. Asim Mansha
Dept. of Chemistry, GCUF

Prof. Dr .Farooq Anwar Dept. of Food Science and Technology, University of Putra Malaysia

Prof. Dr. Tahir Mehmood, Dept. of Microbiology and Molecular Genetics, University of Punjab

Dr. Awais Ahmed Haral
Assistant Professor
Dept. of Chemistry University of Lahore

Prof. Dr. Ameer Fawad Zahoor
Dept. of Chemistry GCUF

Prof. Dr .Faisal Mahmood, Director Campus, Superior University Faisalabad

Dr. Mumtaz Khan
Principal Research Specialist at the China National Nuclear Corporation

Prof. Dr. Irshad Hussain
Syed Babar Ali School of Science and Engineering, LUMS

Prof. Dr. Hassan Syaad Ghulam Ishaq Khan Institute of Science & technology

Prof. Dr. Matloob Ahmed
Dept. of Chemistry, GCUF

Prof. Dr. Abdullah Ijaz Hussain
Dept. of Chemistry GCUF

Dr. Yasir Jameel
Associate Professor,
Dept. of Physics (UAF)

Dr Saba Jameel
Associate Professor
Dept. of Chemistry, UAF

Dr. Muhmmad Adnan Iqbal
Associate Professor,
Dept. of Chemistry, UAF

Dr. Saima Rehman
Associate Professor
Dept. of Chemistry, GCUF.

Dr. Faiz-UR- Rehman
Associate Professor
Dept. of Biochemistry, UOS

Prof. Dr Mudassir Iqbal
Dept. of Chemistry school of natural sciences (SNS), National University of Sciences & Technology (NUST)

Dr Kashif Iqbal
Assistant professor
Dept. of Textile Engineering
NTU Faisalabad

Dr. Amjad Farid
Assistant Professor
Dept. of Physics, GCUF

Dr. Ahsan Nazire, Assistant Professor, Director Oric, NTU Faisalabad

Dr Hammad Majid
University of Management and Technogy, Sialkot

Dr. Muhammad Farooq Principal Scientist
Bioinformatics lab, NIBGE

Prof Dr Khurram Saleem Joya
Department of Chemistry
University of Madinah, Saudi Arabia

Dr. Rabia Faridi
Assistant Professor
Dept. of Plant Breeding & Genetics, UAF, Faisalabad.

Dr. Asma Rehman Principal Scientist, Nanobiotechnology group at IBD, NIBGE

Dr. Kiran Aftab
Associate Professor Dept. of Chemistry GCUF

Dr. Ayesha Younas
Associate Professor Dept. of Physics GCWUF

Dr. Sumaira Naeem
Assistant Professor Dept. of Chemistry Baba Guru-Nanak University

Conference Program, 4-th December 2024, Day-I

Timeline		
Inauguration **Jinnah Auditorium, GCWUF** **09:00-09:30 am PST**		
09:00-09:30am	Recitation from the Holy Quran by Ms Maham IJaz Naat-e-Rasool e Maqbool by Ms Hira Rafique Welcome note by Dr Abida Kausar, Chairperson Department of Chemistry GCWUF Remarks by Chief Guest, Prof Dr Rauf-e-Azam, Vice Chancellor, GC University Faisalabad. Address by Patron in Chief, Prof Dr Kanwal Ameen (T.I.), Vice Chancellor GCWUF Welcome note by Prof Dr Zill-I-Huma Nazli, Pro-Vice Chancellor, GCWUF Distribution of Shields/Certificates	
Plenary Lecture **Jinnah Auditorium, GCWUF** **09:30-10:40 am PST**		
09:30-10:10am	Prof Dr Mark G. Molony. Professor Emeritus, Department of Chemistry, University of Oxford. Chemistry and its Applications at a Surface	1
10:10-10:40am	Prof Dr Muhammad Akhyar Farrukh, Dean Faculty of Science and Technology, University of Central Punjab, Lahore. Sustainable Graphene-Based Nanomaterials for Environmental Solutions	2
Tea Break & Poster Session **Apron Lawn of Jinnah Auditorium, GCWUF** **10:40-11:20 am PST**		
Session Convener: Dr Maryam Aslam, Dr Umme Kalsoom		

Session-I: Natural & Synthetic Medicinal and Pharmaceutical Sciences by Integrated Computational Approach

Committee Room, GCWUF

11:20 am-01:40 pm PST

Chair: Prof Dr Fazli Rabbi Awan, Principal Scientist, Health Biotechnology Division, NIBGE, Faisalabad.

Co-Chair: Prof Dr Tahir Mehmood. Institute of Microbiology and Molecular Genetics, University of Punjab Lahore

Session Convener: Dr Nusrat, Dr Shagufta Parveen, Dr Maryam

	Activity of Heterocyclic Compounds	
01:30-01:40 pm	Sabra Ikhlas, Department of Chemistry, GC Women University Faisalabad. Recent Advances in the Piperazine based Antiviral Agents: A Remarkable Heterocycle for Antiviral Research	11
Session II: Interdisciplinary Research Trends **Jinnah Auditorium, GCWUF** **11:20 am-01:30 pm PST**		
Chair: Prof Dr Asim Mansha, Department of Applied Chemistry, GC University Faisalabad Co-Chair: Prof Dr Matloob Ahmed, Department of Applied Chemistry, GC University Faisalabad Session Convener: Dr Sana Aslam, Dr Sadia Asim, Dr Farhat Jubeen		
11:20 - 11:40 am	Invited Talk: Prof Dr Asim Mansha, GC University Faisalabad. Theoretical exploration of optoelectrical properties of photocatalytic metal compounds, a case study of Metal Vandate Oxide	13
11:40-12:00 pm	Invited Talk: Prof Dr Matloob Ahmed, GC University Faisalabad. Benzothiazines and Benzimidazoles as anti-diabetic agents: Synthesis & biological activity	14
12:00-12:20 pm	Invited Talk: Prof Dr Ameer Fawad Zahoor, GC University Faisalabad. Epoxide Ring Opening Reactions: Gateway to Unnatural Amino Acids and Biologically Potent Molecules	15
12:20-12:40 pm	Invited Talk: Prof Dr Muhammad Hassan Sayyad, Department of Physics, GIK institute of Engineering Sciences. Light-Matter Interaction Physics: Unraveling the Potential for Research, Medical Innovations, and Industrial Advancements	16
12:40-01:00 pm	Invited Talk: Dr Hammad Majeed. Director ORIC, University of Management and Technology, Sialkot., Interdisciplinary Collaborative Research Techniques for Sustainable Industrial Applications to Enhance Societal Impact and Profitability	17
01:00-01:10 pm	Dr. Shumaila Kiran. GC University Faisalabad. Synthesis and characterization of bio-fabricated silver nanoparticles as green catalysts for mitigation of synthetic dyes: A sustainable environmental remedial approach	18
01:10-01:20 pm	Zill-e-Huma, Interdisciplinary Research Center in Biomedical Materials, COMSATS Lahore Campus, Islamabad. A novel and Universal Functionalized Hazo-POPs@COOH-Apt/PGE-based Electrochemical Biosensor for Detection of Aflatoxins M_1 (AFM_1) in Raw Milk sample: A Versatile Peroxidase-Mimicking Aptananozyme	19

	Approach	
01:20- 01:30 pm	Sumayya Akram. Department of Chemistry, GC University Faisalabad. Exploring N-Arylation of Pyrazoles: Synthetic Routes and their Biological Applications	20
Lunch break **Apron Lawn of Jinnah Auditorium, GCWUF** **01:45-02:30 pm PST**		
Session III: Emerging Technologies in Environmental Sciences **Jinnah Auditorium, GCWUF** **02:30-05:20 pm PST**		
Chair: Prof Dr Haq Nawaz Bhattii, University of Agriculture Faisalabad Co-Chair: Dr Kiran Aftab, Department of Chemistry, GC University Faisalabad Session Convener: Dr Abida Kausar, Dr Umme Kalsoom, Dr Nadia Noor		
02:30- 02:50 pm	Invited Talk: Prof Dr Amjad Farid, Department of Physics, GC University Faisalabad. Hierarchical Nanostructures on 3D Porous Frameworks for Sensing Applications	21
02:50- 03:10 pm	Invited Talk: Prof Dr Khurram Saleem Joya, Department of Chemistry, University of Madinah, Madinah, Saudi Arabia. Synthetic Fuels: Innovative Materials for energy conversion and Storage	22
03:10- 03:30 pm	Invited Talk: Dr Mumtaz Khan, Principal Research Specialist. China National Nuclear Cooperation. Emerging Technologies in Environmental Sciences: A paradigm Shift in sustainable Solutions	23
03:30- 03:50 pm	Invited Talk: Dr Umer Shafique, Department of Chemistry, GC University, Lahore. Perfluoroalkyl Acids: Emerging Pollutants in the Environment	24
03:50- 04:00 pm	Dr Noshin Afsha, Shandong Cancer Hospital and Institute, Shandong First Medical University & Shandong Academy of Medical Sciences, China. Enzyme-free Isothermal Amplification Dual-Target DNA Biosensors for Early Metastatic Breast Cancer Diagnosis	25
04:00- 04:10 pm	Ayesha Yousaf, Department of Chemistry, GC Women University, Sialkot. Photocatalytic activity of Bi Doped CuO-rGO Nanocomposite for Removal of Crystal Violet Dye	27
04:10- 04:20 pm	Tuba Irtaza, Department of Chemistry, GC University Faisalabad. Electro-Oxidation of strontium Tungstate Fabricated Graphitic Carbon Nitride for Hydrogen Production via Water Splitting	28

04:20-04:30 pm	Muqadas, Department of Chemistry, GC University Faisalabad. Electro-Oxidation of Stannous Tungstate Fabricated Graphitic Carbon Nitride for Hydrogen Production via Water Splitting	29
04:30-04:40 pm	Esha Ismail, Department of Chemistry, GC University Faisalabad. Study of polyacrylamide mediated peanut shell/alumina ternary composite for removal of dyes from water	30
04:40-04:50 pm	Malaika Razzaq Khan, Department of Chemistry, GC Women University Sialkot. Removal of Dyes by Bimetallic Nanoparticles incorporated onto Metal Organic Framework: A Sustainable Approach	31
04:50-05:00 pm	Sana Ijaz, Department of Chemistry, GC Women University, Faisalabad. Synthesis and Application of Rice Husk Derived Cellulose Composite with Graphene Oxide as Potentially Effective Adsorbent for Dyes Removal	32
05:00-05:10 pm	Hafsa Saleem, Department of Chemistry, GC Women University Faisalabad. Recent synthetic strategies of medicinally important imidazothiadiazoles	
05:10-05:20 pm	Eman Fatima, Department of Chemistry, GC Women University, Faisalabad. Eco-Innovation: Green Synthesis of Silver Nanoparticles from Agriculture Byproducts	

Session-IV: Nano-Chemistry & Nano-Technology Applications

Committee Room, GCWUF

02:30-05:20 pm PST

Chair: Prof Dr Yasir Jamil, Department of Physics, University of Agriculture Faisalabad

Co-Chair: Dr Muhammad Adnan Iqbal, Department of Chemistry, University of agriculture, Faisalabad

Session Convener: Dr Maryam Aslam, Dr Faiza Nazir, Dr Huma Munir

02:30-02:50 pm	Invited Talk: Dr Yasir Jamil, Department of Physics, University of Agriculture, Faisalabad. Green Laser Assisted Synthesis and Photocatalytic Innovations with Gold-Cobalt Nanoparticles	
02:50-03:10 pm	Invited Talk: Dr Saima Rehman, Department of Chemistry, GC Women University, Faisalabad. Mxenes based Nanostructures for Electrochemical Sensing	32
03:10-03:30 pm	Invited Talk: Dr Saba Jamil, Department of Chemistry, University of Agriculture Faisalabad. Carbon Nanodots and its Modification and	33

	Applications	
03:30-03:50 pm	Invited Talk: Dr Faisal Mehmood, Director Academics, Superior University, Faisalabad Campus. Nanotechnology for Sustainability: Bridging Innovation and the SDGs	36
03:50-04:10 pm	Invited Talk: Dr Rabia Faridi, Department of Plant Breeding and Genetics, University of Agriculture, Faisalabad. Nanoparticle-Induced Systemic resistance in Mungbean against Yellow Mosaic Virus	35
04:10-04:30 pm	Invited Talk: Dr Muhammad Adnan Iqbal, Department of Chemistry, University of agriculture, Faisalabad. Exploring Selenium-N-Heterocyclic Carbene Compounds and Nanoparticles: A Synergy of Synthesis, Computational, and Biological Assessments	34
04:30-04:50 pm	Invited Talk: Dr Ahsan Nazir, Director ORIC, NTU, Faisalabad. Electrospun Nanomaterials for Biomedical Applications	
04:50-05:00 pm	Hafiz Affan, Department of Textile Engineering, National Textile University, Faisalabad. Application of Highly Abrasion Resistant Functional Coatings on Cotton Fabric	
05:00-05:10 pm	Amna Kashif, Department of Chemistry, GC Women University, Faisalabad. Eco-Inspired Nanoparticles: Rice Husk-Derived Zinc Oxide for promoting Coriander Growth	
05:10-05:20 pm	Rimsha Kanwal, Department of Chemistry, University of Agriculture Faisalabad. Synthesis of N-Alkyl Azoles Carrying Metal Complexes for Catalytic and Medical Applications	

Conference Program, 5th Dec-2024, Day-II

Timeline		
Jinnah Auditorium, GCWUF **09:00-09:15 am PST**		
09:00-09:15 am PST	Recitation from the Holy Quran Ms Maham Ijaz Naat-e-Rasool e Maqbool by Ms Sana Rehmat	
Plenary Lecture **Jinnah Auditorium, GCWUF** **09:15-09:55 am PST**		
09:15-09:55 am	Dr. Awais Ahmed, Assistant Professor, University of Lahore, Benign-by-Design Preparation of Nanomaterials for Catalytic and Sustainable Applications	37
Tea Break **Apron Lawn Jinnah Auditorium, GCWUF**		

09:55-10:30 am PST	
Session V: Training Workshop on Data Analysis **Jinnah Auditorium, GCWUF** **10:30am -01:35 pm PST**	
10:30am - 12:15 pm	Prof Dr Khurram Saleem Joya, Department of Chemistry, University of Madinah, Madinah, Saudi Arabia. • Data management of SEM, EDS, XPS • Handling and data interpretation of Electrochemical research tools CV, LSV, EIS/impedance, SWDPV, Anodisation, Electrodeposition, ECSA, Tafel
12:15pm - 01:05 pm	Dr Faiz-Ur-Rehman, Associate Professor, Department of Biochemistry, University of Sargodha. Intro to AI + Writing, Drafting and Editing Tools
Lunch break **Apron Lawn of Jinnah Auditorium, GCWUF** **01:05-01:50 pm PST**	
Session VI: Training Workshop **Jinnah Auditorium, GCWUF** **01:50-4:20 pm PST**	
01:50-02: 50 pm	Dr Faiz-Ur-Rehman, Associate Professor, Department of Biochemistry, University of Sargodha. Literature Search and Review, Citation and reference management and Ethics
02:50-04: 20pm	Dr Muhammad Farooq, Principal Scientist, NIBGE, Faisalabad. • NGS based Assembly and Annotation of Bacterial Genomes Sequencing Data on the Free Galaxy Platform. • Data Analysis Tools on Galaxy incl. FASTQC / MultiQC / QUAST / SPADES / PROKKA
Dinner **Sports Ground, GCWUF** **06:30-8:30 pm PST**	

Conference Program, 6th Dec-2024, Day-III

Timeline

Jinnah Auditorium, GCWUF **09:00-08:15 am PST**		
09:00- 09:15 am	Recitation from the Holy Quran Ms Maham Ijaz Naat-e-Rasool e Maqbool by Ms Sana Rehmat	
Plenary Lecture **Jinnah Auditorium, GCWUF** **09:15-11:10 am PST**		
09:15- 09:55am	Plenary Lecture: Halil İbrahim ULUSOY, Department of Analytical Chemistry, Faculty of Pharmacy, Sivas Cumhuriyet University, Türkiye. Collaboration of Material Science and Conventional Instrumental Analysis for Sensitive Analysis of Drug Molecules	38
09:55- 10:35 am	Plenary Lecture: Prof Dr Shazia Anjum, Vice Chancellor, The Islamia University of Bahawalpur, Economics of Panoramic Drug Discovery of Natural Products	39
10:35- 11:15 am	Prof. Dr. Irshad Hussain. Professor & Department Chair, Department of Chemistry & Chemical Engineering, School of Science & Engineering (SSE), Lahore University of Management Sciences. Functional Nanomaterials-Tuning the Size and Surface Chemistry for Applications in Biomedical Science, Renewable Energy Technologies and Environmental Remediation	40
Closing **Jinnah Auditorium, GCWUF** **11:15-11:45 am PST**		
	Distribution of Souvenirs Vote of Thanks by Dr Abida Kausar, Chairperson, Department of Chemistry, GCWUF Vote of Thanks by Prof Dr Zill I Huma Nazli, Patron, Pro-Vice Chancellor, GCWUF Remarks by the Chief Guest Remarks by the Guest of Honour Remarks by Prof Dr Kanwal Ameen (T.I.), Patron-in-Chief, Vice Chancellor, GCWUF Group Photo	
Tea & Jumma Prayer Break **Apron Lawn of Jinnah Auditorium, GCWUF** **11:45am -01:30 pm PST**		
Session VII: Frontiers in Nutrition: Food Chemistry **Committee Room, GCWUF** **01:30 -03:50 pm PST**		
Chair: Prof Dr Kaleem Khosa, Department of Chemistry, GC University Faisalabad		

Session Convener: Dr Rehana Naseer, Dr Nazia Yaqoob		
01:50-02:10 pm	Invited Talk: Prof Dr Ameer Kashif. University of Sargodha Green Extraction Techniques for Clean Label Recovery of Polyphenols from Plant Sources	40
02:10-02:30 pm	Invited Talk: Prof Dr Farooq Anwar, Emerging Trends in the Extraction of Bioactive Ingredients from Selected Fruits, Oil Seed and Agro-wastes	41
02:30-02:40 pm	Syed Ali Hassan Shah, Department of Chemistry, University of Agriculture, Faisalabad. Antidiabetic activity-based fortification of olive and Mustard oils using Mangifera Indica (Neem) and Fagonia Indica Plant Extracts	42
02:40-02:50 pm	Neelam Iftikhar, Department of Chemistry, GC University Faisalabad. Effects of Polyphenol-Rice Hisbiscus and Zingber Teas on Obesity and Oxidative Stress in Rats Fed a High-Fat-Sugar Diet	43
02:50-03:00 pm	Iqra Kanwal, Department of Chemistry, University of Agriculture, Faisalabad. Exploration of Antidiabetic and Antioxidant Potentials of *Morus* Leaves	44
03:00-03:10 pm	Maheen Almas, Department of Chemistry, GC University Faisalabad. Development of Multifunctional Bioactive Food Packaging based on Silver Nanoparticles/Grape Fruit Peel Extract Reinforced PVA Composites	45
03:10-03:20 pm	Dr Shaista Rafique, Department of Physics, Government College Women University, Faisalabad. Facile fabrication of Novel Silver-Polypyrrole-Multiwall Carbon Nanotubes nanocomposite for Replacement of Platinum in Dye-Sensitized Solar Cells	46
03:20-03:30 pm	Faiza Safdar, Department of Textile Engineering, National Textile University Faisalabad.Synthesis of modified TiO_2 nanoparticles for the development of multifunctional substrate	47
03:30-03:40 pm	Naz Tehreem, Department of Chemistry, University of Education Lahore, Faisalabad Campus. Unveiling the Solubilization Behavior of Nickel, Cobalt and Zinc Fluoride Complexes in Micellar Media of Sodium Lauryl Sulphate by Conductometery, UV/Vis and 1H-NMR Spectroscopy	48
03:40-03:50 pm	Rahila, Department of Chemistry, University of Education Lahore, Faisalabad Campus. 1H-NMR and DLS Study of Formulated Microemulsion System Emulsified with Non-ionic Surfactant	49
Session VIII :Smart & Sustainable Development in Materials Manufacturing and Energy **Jinnah Auditorium, GCWUF**		

01:30 -03:50 pm PST		
Chair: Prof Dr Kaleem Khosa, Department of Chemistry, GC University Faisalabad Session Convener: Dr Sadia Nazir, Dr Faiza Amin, Dr Nadia Noor		
01:30- 01:50 pm	Invited Talk: Prof Dr Mudassir Iqbal, Department of Chemistry, School of Natural Sciences (SNS), National University of Science and Technology, Islamabad. MEXENES as Versatile Materials for Energy Applications	50
02:10- 12:30 pm	Invited Talk: Dr Kiran Aftab, Associate Professor, Department of Chemistry, GC University, Faisalabad. Upcycling of PET Waste into Interfacial Solar System Generators: Advances and Challenges	51
02:30 - 02:50 pm	Invited Talk: Dr Arifa Jamil, Department of Physics, GC Women University Faisalabad. Effect of Titanium Doping on Conductivity, Density of States and Conduction Mechanism in ZnO thin film	52
02:50- 03:10 pm	Invited Talk: Dr Ayesha Younas, Department of Physics, GC Women University, Faisalabad. Applications of Terahertz Systems for Non-Destructive Evaluation of Emerging Materials in Science and Industry	
03:10- 03:30 pm	Invited Talk: Dr Kashif Iqbal, Department of Textile Engineering, National Textile University Faisalabad. Innovation in Textile Chemistry and Approach towards Sustainability	
03:30- 03:40 pm	Dr Shamsa Bibi, Department of Chemistry, University of Agriculture, Faisalabad. Innovative Computational Approaches for Designing Advanced Optoelectronics Materials towards Energy Applications	53
03:40- 03:50 pm	Sameen Maqsood, Department of Physics, University of Agriculture, Faisalabad. Optimization of 3C-SiC and CdS Electron Transport Layers for Enhanced Performance in Sb2S3-based Solar Cells: A SCAPS-ID Simulation Approach	54

ABSTRACTS

Chemistry and its Application at a Surface

Moloney, M. G.*

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Abstract:

We have extensively developed diaryldiazo reagents as carbene precursors suitable for chemical reactions at a surface, leading to covalent bond formation, and introducing a range of properties that can be detected at a macroscopic level; these include colour, fluorescence, hydrophobicity and hydrophilicity, wettability, metal chelation and biocidal properties. More recent work has shown that bis-(diaryldiazo) reagents are both easily prepared and handled, but show excellent reactivity at a surface, and importantly with appropriate substitution, allows a combination of both surface reaction and intramolecular cross-linking. This has been used to bind the enzyme cellulase by direct capture without loss of activity, and to modify gold electrodes and change electrochemical behaviour. A discussion of some of the underlying chemistry attempts to explain why these reagents are so effective for surface modification; un-solvated solid state reactions at the surface appear to be crucial for the success of this approach.

Sustainable Graphene-Based Nanomaterials for Environmental Solutions

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Abstract:

The green synthesis of nanomaterials, utilizing various biological sources such as plants and microorganisms, offers a sustainable and eco-friendly approach to minimize toxic waste generation. In our study, we synthesized over 70 nanocomposites incorporating graphene derivatives—namely, graphene oxide (GO) and reduced graphene oxide (rGO)—along with p, d, and f block metals/metal oxides and their nanocomposites. These were prepared using plant extracts and microbial processes through two distinct green methods: a one-pot green synthesis and a green deposition method. The resulting nanocomposites were designed for applications in the degradation of pollutants from textile, pharmaceutical, pesticide, fertilizer, and chemical industries. Graphene has gained significant attention due to its exceptional properties and broad application potential, making it one of the most promising nanomaterials. Derivatives like GO and rGO, obtained from graphite through various synthesis methods, differ primarily in their carbon-to-oxygen ratio, surface area, dispersibility, hydrophobicity, and electrical conductivity. Further modification of GO and rGO surfaces with metal and metal oxide nanoparticles enhances their chemical and biological properties, making them highly effective in removing environmental pollutants from chemical and pharmaceutical wastewater.

Plants: A Vital Source of Nutraceuticals and Functional Foods

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Abstract:

The usage of functional foods and nutraceuticals is becoming more popular due to recent advancements in the field of optimal nutrition. A concentrated or isolated portion of a naturally occurring food that is high in nutrients is called a nutraceutical, and it is supplied in medical forms such tablets, capsules, and ampules, among others. They contain ingredients that aren't typically thought of as nutrients yet have beneficial physiological effects that help prevent chronic diseases. Nutraceuticals are referred to by many names in different countries, including phytochemical-rich foods, functional foods, designer foods, and natural health supplements. Numerous bioactive substances and high-value constituents, including biopeptides, carotenoids, , essential fatty acids, dietary fiber, isothiocyanates, flavonoids, polyols, plant stanols/phytosterols, phytoestrogens, prebiotics/probiotics, soy protein, sulfides/thiols, etc., are responsible for the physiological and medicinal health benefits of nutraceuticals. They are used to treat a wide range of illnesses, enhance well-being, slow down the ageing process, avoid chronic illnesses (diabetes, cancer, viral infections, etc.), lengthen life expectancy, maintain the body's structural integrity, and regulate gene expression. The primary bioactive substances found in nutraceuticals are secondary metabolites, or plant-based molecules with therapeutic effects. The World Health Organization has acknowledged the potential of nutraceuticals as a safer, more focused, and more effective treatment for a number of common diseases, such as obesity, hypertension, cancer, diabetes, viral infections, and cardiovascular disorders. Nevertheless, there is an urgent need to clarify the molecular mechanisms underlying the actions of these beneficial products. The idea, classification, and possible medical and therapeutic uses of several commercially available nutraceuticals are the main topics of this presentation. It also highlights the current trends, issues, and opportunities facing the nutraceutical sector.

Designing Functionalized Nanomaterials for Biomedical and Environmental Applications

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Abstract:

Functionalized nanomaterials such as silver, zinc, gold and copper have consistently and completely revolutionized the biomedical and environmental science for the last few decades. The unique structural and optical properties at nanoscale empower the development of novel nanomaterials as promising catalyst, drug carriers, and antimicrobial agents. This talk will comprehend the surface tuning of nanoparticles with biomolecules (phytochemicals, biosurfactant etc) in order to enhance their interaction with bacterial and animal cells and boost their therapeutic efficacy. For this purpose, Surfactin conjugated silver nanoparticles (SC@AnGPs) were synthesized as efficient antibacterial and antibiofilm nano-biotics against antibiotic resistant bacteria (Pseudomonas aeruginosa) for safe dermal applications. Additionally, this talk will cover the environmental applications of developed nanomaterial including fabrication and application of visible light driven photocatalysts, conversion of biowaste into value added nanomaterials. The management of large biological waste is a global problem as it is dumped openly at landfills with odor production and microbial growth. This waste management concern has paved the way towards the use of biowastes for production of value-added nanomaterials, functionally important in diverse applications. The current study focused on the conversion of egg shells to hydroxyapatite (HAP) using a sustainable procedure and explored its applications as potent adsorbent for lead removal. Further the functionalized nanomaterials were used as efficient photocatalyst for degradation of toxic CBB dye with ~90% degradation efficiency.

Medicinal Plants and Non-Communicable Diseases (NCDs): Utilization of Multidirectional Approach Probe into the New Nutraceuticals

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Abstract:

Medicinal herbs have been used for centuries to prevent and manage non-communicable diseases (NCDs). NCDs, such as heart disease, stroke, diabetes, cancer, and chronic respiratory diseases, are the leading causes of death globally. There are some medicinal herbs and their potential benefits in preventing and managing NCDs; Ashwagandha (Withania somnifera): Enhances immune function, reduces inflammation, and inhibits cancer cell growth. Further Reduces stress, anxiety, and improves cognitive function. Nepeta species are also characterized by a wide range of uses in folk medicinal system like antimicrobial, insect repellent, insecticide, larvicide, cytotoxic anticarcinogen, antioxidant, anticonvulsant, analgesic, anti-inflammatory agent, and antidepressant. Owing to the medicinal importance of these plants, the present work was planned to determine complete phytochemical composition, antioxidant potential and enzyme inhibition properties of the various extracts, which were subjected to the measurement of their phenolic and flavonoid contents, whereas, to unveil the complete secondary metabolic picture, the total methanolic extract was analyzed by HPLC-MS. Various bioassays (DPPH, CUPRAC, ABTS, FRAP, Phosphomolybdenum and metalchelation assays) were performed to measure antioxidant potential of the extracts, whereas, the extracts were also evaluated against key enzymes involved in common ailments like diabetes (α-glucosidase and β-amylase) neuro-degenerative disorder (AChE and BChE) and skin problems (tyrosinase). Statistical and docking studies were also performed to highlight possible interaction between the bioactive content and tested biological assays.

Engineering and Physiochemical Characterization of Nanostructured Liposomes based Red Blood Cells-Mimics as Smart Carriers for Drug Delivery Applications

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Abstract:

Liposomes based red blood cells-mimics (RBCMs) which can mimic certain characteristics of the red blood cells (RBCs) were synthesized by using the thin-film hydration technique to address problems faced in targeted drug delivery systems. These liposomes based RBCMs were synthesized by using the phosphatidylcholine (PC) phospholipid formulated in the presence of emulsifiers of Tween®80 and dicetyl phosphate (DCP). Other phospholipids including dipalmitoylphosphatidylcholine (DPPC), distearylphosphatidylcholine (DSPC), phosphatidylserine (PS), and L-a-phosphatidylinositol (PI) were also used in different combinations to impart electrical and morphological characteristics of RBCs to the synthesized liposomes. The physicochemical characterization of the engineered liposomes was performed by using optical polarizing microscopy (OPM), transmission electron microscopy (TEM), field emission scanning electron microscopy (FESEM), dynamic light scattering (DLS), and differential scanning calorimetry (DSC). Our research group was successful in synthesizing the RBCMs with the mean particle size of 70-80 nm which is in accordance with the size of RBCs. Moreover, the zeta potential of -3 mV to -14mV (well within the range of zeta potential of RBCs) was successfully mimicked as well. Drug encapsulation efficacy of the RBCMs for numerous drugs was further investigated and the stability studies of the drug loaded RBCMs were performed for investigating the practical applicability of the synthesized RBCMs. The results affirmed that the synthesized RBCMs exhibited long term stability at the temperature

values of 4 (freezer based storage temperature), 28 (room temperature) and 37 (physiological temperature) for 28 days. Acquired findings revealed that the synthesized RBCMs exhibit excellent potential for *in vitro* anti-cancer drug delivery applications.

Fabrication and Kinetic Evaluation of Dye Adsorption Capability of Metal Oxide@Rgo Nanocomposites Integrated Cellulose Triacetate Membranes

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Abstract:

Reduced Graphene Oxide (RGO) and its derivatives exhibit remarkable removal abilities of water pollutants that can further be enhanced by the incorporation of the metallic nanoparticles. However, the challenging collection of GO sheets and fabrication method of RGO-based materials during the adsorption process, constraint their practical uses. The integration of the RGO-based materials on the polymeric matrix offers a solution to this problem. In current study, three types of metal oxide@RGO nanocomposites integrated Cellulose Triacetate (CTA) membranes with adsorption abilities were prepared by a facile blending and phase inversion technique. The fabricated membranes exhibited selective adsorption for azo dyes at room temperature. The adsorption parameters depicted the Langmuir and pseudo-first order kinetic order reaction. It was found that the adsorption process was directed by the inter-particle diffusion. These membranes were found to be effective against varying range of the pollutants and can be fabricated by the facile techniques.

Highly Efficient Aramid Fiber Supported Polypropylene Membranes Modified with Reduced Graphene Oxide based Metallic Nanocomposites: Antimicrobial and Antiviral Capabilities

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Abstract:

Polypropylene hybrid polymeric membranes with aramid support have been fabricated using Thermally Induced Phase Separation (TIPS). Different modifying materials, such as metallic nanoparticles and reduced graphene oxide (rGO), improve the properties of these membranes. The nanomaterials and the fabricated membranes have been characterized with FTIR spectrometer, SEM and UV-Vis Spectrophotometer. Following that, the disinfection capabilities of the fabricated hybrid membranes were investigated. The antibacterial capability of the membranes is established through the testing of the membranes against bacterial strains *S. aureus* and *E. coli*, whereas the antiviral evaluation of the membranes was made against *H9N2* and *IBV* strains. This research aims to develop advanced hybrid membranes that effectively disinfect water by incorporating novel nanomaterials and optimizing fabrication techniques.

A Comprehensive Update of Anti-COVID-19 Activity of Heterocyclic Compounds

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Abstract:

The Coronavirus disease 2019 (COVID-19) pandemic is one of the most considerable health problems across the world. Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) is the major causative agent of COVID-19. The severe symptoms of this deadly disease include shortness of breath, fever, cough, loss of smell, and a broad spectrum of other health issues such as diarrhea, pneumonia, bronchitis, septic shock, and multiple organ failure. Currently, there are no medications available for coronavirus patients, except symptom-relieving drugs. Therefore, SARS-CoV-2 requires the development of effective drugs and specific treatments. Heterocycles are important constituents of more than 85% of the physiologically active pharmaceutical drugs on the market now. Several FDA-approved drugs have been reported including molnupiravir, remdesivir, ritonavir, oseltamivir, favipiravir, chloroquine, and hydroxychloroquine for the cure of COVID-19. In this study, we discuss potent anti-SARS-CoV-2 heterocyclic compounds that have been synthesized over the past few years. These compounds included; indole, piperidine, pyrazine, pyrimidine, pyrrole, piperazine, quinazoline, oxazole, quinoline, isoxazole, thiazole, quinoxaline, pyrazole, azafluorene, imidazole, thiadiazole, triazole, coumarin, chromene, and benzodioxole. Both in vitro and in silico studies were performed to determine the potential of these heterocyclic compounds in the fight against various SARS-CoV-2 proteins.

Recent Advances in the Piperazine based Antiviral Agents: A Remarkable Heterocycle for Antiviral Research

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Abstract:

A growing interest in pharmacology has made heterocyclic chemistry as one of the emerging branches of organic chemistry. Piperazine is an excellent heterocycle that possesses a large span of pharmaceutical applications. Piperazine derived compounds have shown multiple therapeutic activities such as antioxidant, antibacterial, analgesic, anticancer, antihypertensive, anti-allergic, anti-inflammatory, antimalarial, antipsychotic, cardioprotective, antifungal, antidepressant and antiviral. FDA has approved many piperazine scaffold-based drugs for the treatment of various viral infections, therefore establishing the pharmacological importance of piperazine derivatives. Only a few reviews on antiviral activities of piperazine containing compounds are available in the literature, despite of its great medicinal significance.

Recent Synthetic Strategies of Medicinally Important Imidazothiadiazoles

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Abstract:

Imidazothiadiazole is a fundamental fused heterocyclic compound containing imidazole and thiadiazole ring systems. This versatile framework has significant applications in pharmaceutical chemistry and also possessed a remarkable biological profile. The derivatives of imidazo [2,1-b][1,3,4]thiadiazole have a broad spectrum of biological applications such as antitumor, tubulin inhibitor, anticancer, antifungal, anti-inflammatory, antimicrobial, antitubercular, anticonvulsant, antibacterial and as enzyme inhibitors. These derivatives also play a significant role in the development of non-linear optics and photo-electronics. Synthesis of this fused bicyclic compound mainly involved the reaction between 2-amino-1,3,4-thiadiazoles and a-haloketones, with different substitutions at the 2, 5, and 6 positions of the ring system. Moreover, microwave assisted multicomponent and C–C coupling reactions in the presence of catalysts or under solvent free reaction conditions were found to be reliable and valuable approaches. This review is a concerted approach to describe the synthesis and applications of imidazo-[2,1-b][1,3,4]thiadiazole derivatives.

Theoretical Exploration of Optoelectrical Properties of Photocatalytic Metal Compounds: A Case Study of Metal Vandate Oxide

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Abstract:

The semiconducting properties of many metal oxide compounds make them suitable candidates for the application as a photocatalyst. When they are exposed to light, electron whole pairs are generated that lead them to act as photocatalyst as degrading organic pollutants and in wastewater treatment. Theoretical investigations based on the first principles density function of structural, thermodynamic and optical properties of this metal oxide is an efficient tool to design new metal oxides having remarkable properties of a photocatalyst. These investigations are performed within generalized gradient approximation (GGA) via ultrasoft pseudopotential and density functional theory method (DFT). The electronic structure is analyzed with a focus on the nature of the electronic states near the band edges. The metal oxides of vendates like K_3VO_4, Na_3VO_4, and $Zn_3V_2O_8$ are investigated for their photocatalytic properties for water splitting. Electronic band structure revealed that among Fe and Co, 6% Co significantly tunes the band gap with the emergence of new states at Gamma point. Notable variations have been highlighted in the electronic properties of $Na_3V_{(1-x)}Fe_xO_4$, $Na_3V_{(1-x)}Co_xO_4$ $K_3V_{(1-x)}Fe_xO_4$, $K_3V_{(1-x)}Co_xO_4$, $Zn_{3(1-x)}V_{2(1-x)}Co_xO_8$ and $Zn_{3(1-x)}V_{2(1-x)}Fe_xO_8$ (where x=0.06) due to different nature of unoccupied 3d states of Fe and Co. Density of states analysis as well as (spin up) and (spin down) magnetic moments showed that cobalt can reduce the band gap by positioning the valence band higher than O 2p orbitals and the conduction band lower than V 3d orbitals. Elastic properties including bulk modulus, shear modulus, Pough ratio and Poisson ratio computed $Zn_3V_2O_8$ to be mechanically more stable than Na_3VO_4 and K_3VO_4. Theoretical investigations will open up a new line of exploration into the photocatalytic characteristics of ortho-vanadates.

Benzothiazines and Benzimidazoles as Anti-Diabetic Agents: Synthesis & Biological Activity

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Abstract:

α-Glucosidase inhibitors (AGIs) play a crucial role for the treatment of diabetes mellitus. The α-Glucosidase enzyme performs its function in the body in breaking down the dietry carbohydrates to small sugar molecules that are further helpful in providing energy for routine functions of the body. However, diabetic patients find it difficult to utilize the blood sugar effectively due to insufficient insulin that subsequently results in increased blood sugar levels. AGIs slow down the digestion of carbohydrates and are thus helpful in controlling the diabetes. During our research on the synthesis of heterocyclic compounds belonging to diversified families of organic compounds, we have identified new molecules as effective α-glucosidase inhibitors. The compounds show good to potent inhibition and are therefore interesting for the people working on drugs for diabetes.

Epoxide Ring Opening Reactions: Gateway to Unnatural Amino Acids and Biologically Potent Molecules

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Abstract:

Epoxide ring opening reactions serve as powerful synthetic tools for the synthesis of complex organic molecules. Epoxides can be opened up by a variety of nucleophiles. These reactions have gained much importance due to their application in the synthesis of natural products, heterocycles and biologically active compounds. Herein, ring opening of epoxides with C-nucleophiles, N-nucleophiles and S-nulceophiles have been presented, thereby leading to toward the synthesis of complex amino acids, ciprofloxacin derivatives and beta-hydroxy sulfides just over a few steps.

Light-Matter Interaction Physics: Unraveling the Potential for Research, Medical Innovations and Industrial Advancements

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Abstract:

Light-matter interaction is one of the most fundamental phenomena in physics, shaping not only our understanding of the physical world but also driving some of the most transformative technological and medical innovations of the 21st century. The interplay between light (photons) and matter (electrons, atoms, molecules, and solids) governs a wide range of physical phenomena, including absorption, emission, scattering, and nonlinear effects. The study of these interactions has evolved into a broad and multidisciplinary field, with crucial applications across diverse domains including quantum mechanics, optics, material science, healthcare, and industry. This talk explores the broad spectrum of research developments in light-matter interactions, highlighting their profound impact on both theoretical and applied sciences. By focusing on the latest advancements in quantum optics, medical technologies, and industrial applications, the session will provide an overview of the potential for light-matter interaction to revolutionize research methodologies, medical treatments, and industrial processes. The talk will also emphasize how interdisciplinary collaborations across physics, chemistry, biology, engineering, medicine, and materials science continue to drive innovation in these critical fields.

Interdisciplinary Collaborative Research Techniques for Sustainable Industrial Applications to Enhance Societal Impact and Profitability

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Abstract:

The integration of interdisciplinary research approaches has become an essential means to propel sustainable industrial applications in the face of increasing environmental concerns, global warming and economic uncertainty. To create novel solutions that not only increase industrial efficiency and profitability but also make a substantial contribution to societal well-being, we must investigate the junction of basic, biological, engineering, data science, artificial intelligence, and applied sciences. We must create effective plans for maximizing resource efficiency, minimizing environmental impact, and promoting economic growth by utilizing a variety of approaches from disciplines like materials science, bioengineering, intelligent manufacturing, simulation and computational modeling. Industries can advance sustainable technology and meet international sustainability objectives, such the Sustainable Development Goals (SDGs) of the UN, by encouraging cross-disciplinary collaboration. These methods have increased both profitability and societal effect, demonstrating how science-driven innovation may be used to solve today's problems. Every industry is searching for new and creative ways to cut costs, boost production, improve quality, and achieve net zero carbon emissions and trash. To address domestic issues that affect the global GDP, we must concentrate on import alternatives. Application-driven objectives and fundamental scientific research must be combined to form a synergistic framework for industry's sustainable development. The Nobel Prize winners also work in collaborations to develop something different which can change the world.

Synthesis and Characterization of Bio-Fabricated Silver Nanoparticles as Green Catalysts for Mitigation of Synthetic Dyes: A Sustainable Environmental Remedial Approach

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Abstract:

The greener synthesis of Ag-NPs is an environment-approachable, stable, simple, faster, and cheaper approach. In this study, Ag-NPs were manufactured by Punica granatum (Pomegranate) fruit peel extract. The synthesized silver nanoparticles (Ag-NPs) were defined through spectralanalytical methods like SEM, XRD, FTIR, UV-Visible spectroscopy, etc. Optimal conditions to prepare Ag-NPs were found to be temperature 80 °C, pH 9, reactant ratio 3:5, and 70 minutes contact time/reaction time. The silver nanoparticles were utilized for the degradation of Basic Brilliant Flavine Y-40 (Y-40) and Direct Fast Rose FR Red-227 (Red-227) dyes succeeding the optimization of experimental conditions i.e. dyes concentration, silver nanoparticles Ag-NPs, pH range, amount of hydrogen peroxide and temperature. The aimed dyes were discolored at 41 % and 56 % at 0.04 and 0.03 mg dye concentration, 57 and 65 % at 6 mg and 7 mg amount of nanoparticles, 70 and 72 % at 9 pH, 81 and 80 % at 0.5 M of hydrogen peroxide and 90 and 91 % at 40 and 50 °C for both Y-40 and Red-227 dyes, respectively. The results explained that COD & TOC, toxicity assessment, TSS, EC, and pH removal efficiencies were 85.2 & 87.4 % and 91.2 & 92.3 %, 103 and 102 mg/L, 1105 and 1115 µS/cm and 6.91 for Y-40 and Red-227 dyes correspondingly. The UV and FTIR spectrum & degradation pathway similarly affirmed the degradation of selected dyes. This research work proposes a clean method for ecological restoration from toxins for a clean atmosphere.

A Novel and Universal Dual-Functionalized Hazo-POPs@COOH-Apt/PGE-Based Electrochemical Biosensor for Detection of Aflatoxin M_1 (AFM_1), in Raw Milk Sample: A Versatile Peroxidase-Mimicking Aptananozyme Approach.

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Abstract:

A novel dual-functionalized electrochemical aptasensor was developed for ultrasensitive detection of aflatoxin M_1 (AFM_1) in milk. AFM_1 , is a hydroxylated derivative of aflatoxin B_1 (AFB_1), that poses health risks such as reduced liver function, stunted growth in children, and immunosuppression. With no FDA approved decontamination method, a point-of-care (POC) device for the quick and precise monitoring of AFM_1 in milk is essential. The electrochemical aptananozyme-based biosensor combines the specificity from COOH-functionalized-AFM_1-Aptamer (COOH-Apt) and o-hydroxyazobenzene polymers (Hazo-POPs) as a nanozyme probe at pencil graphite electrode (PGE). Hazo-POPs exhibit electroactive properties as well as enzyme like functionalities (peroxidase activity), independently utilized for AFM_1 detection. The synthesized Hazo-POPs were characterized using different techniques, such as XRD, FTIR, UV-Vis, DLS, Raman spectroscopy and FESEM. In method I, the surface of PGE is modified with Hazo-POPs@COOH-Apt to obtain the best electrochemical response. While, In method II, the peroxidase-like activity of Hazo-POPs was used further to confirm the specificity of the aptananozyme (Hazo-POPs@COOH-Apt/PGE) towards AFM_1 detection by measuring the DPV response of 3,3',5,5'-tetramethylbenzidine (TMB). The designed aptasensor (Hazo-POPs@COOH-Apt/PGE) exhibited a broad linear range (0.005-500nM) and lower LOD 0.004 and 0.003 nM for method I and II respectively, under optimized conditions. It demonstrated exceptional sensitivity, improved reproducibility and stability over three weeks. Practical validation was performed by the detection of AFM_1 in spiked milk samples, yielding recovery (101.21 to 104%).

Exploring N-Arylation of Pyrazoles: Synthetic Routes and their Biological Applications

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Abstract:

N-Arylpyrazoles are fundamental components in the development of biologically active compounds, natural products, pharmaceuticals, and various industrial applications. They are core structural units in various drugs, exhibiting a wide range of biological activities, such as antibiotic, anticancer, antifungal, anti-inflammatory, anticoagulant, analgesic, antipyretic, antidepressant, insecticidal, and hyperglycemic effects. Several synthetic methods have been designed to synthesize *N*-arylpyrazoles, including reactions catalyzed by different metals at both high and room temperature, metal-free reactions, named reactions, multicomponent reactions, and reactions driven by different electromagnetic radiations. Additionally, various ligands have also been identified to facilitate the copper-catalyzed *N*-arylation of pyrazoles under mild conditions and in a shorter timeframe. This presentation provides a comprehensive overview of the synthesis and biological applications of *N*-arylpyrazole derivatives reported between 2019 and 2023.

Hierarchical Nanostructures on 3D Porous Frameworks for Sensing Applications

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Abstract:

Quantitative glucose measurement is of great significance for the effective diabetes management. Non-enzymatic glucose sensors (NEGS), due to affordable cost, direct glucose oxidation, boosting sensitivity, and appealing selectivity, have received considerable research efforts recently. However, several shortcomings such as aggregation, inferior chemical stability and poor electrical conductivity of an electrocatalyst material rigorously degraded the overall electrochemical performance of NEGS. Additionally, the usage of organic binders in the fabrication process of an electroactive material frequently resulted in the blockage of active redox sites, restricting deep electrolyte ions penetration and diffusion of target analyte species. To cope the aforementioned issues, current research work focuses on the construction of binder-free, well-architected and highly efficient NEGS. In this context, glucose sensing probes nanomaterials such as nickel vanadate (Ni3V2O8) nano-sheets (NSs) are anchored on highly conductive carbon nano-coils/Nickel foam (CNCs/NF) frameworks, i.e., to design 3D hierarchical composite nanostructures in terms of achieving synergistic effects and desirable electrochemical performance. Amperometric analysis reveals extremely swift detection time (0.1 s), high detection sensitivity (5214μA mM^{-1} cm^{-2}), favorable detection limit (0.04 μM), prominent anti-interference ability, and efficient long-term storage stability. The developed sensor exhibits appreciable recoveries (93.3 to 103.3 %) regarding the determination of glucose levels in human blood serum samples demonstrating its practical utilization

Synthetic Fuels: Innovative Materials for Energy Conversion and Storage

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Abstract:

With the advent on innovative science, chemical research and technology, nanoscale materials can be engineered and programmed to perform specified function at macro level applications. The innovation in chemical science, nanomaterials, catalysis, and electrochemical processes for Water Splitting has a lead now for solar and chemical energy conversion. These systems can be implemented as surface immobilization along with thin-films for catalytic processes, sensing applications and for energy conversion schemes. We have invented, discovered and developed specialized methods, and exploited various thin-film nanoscale materials for catalytic water splitting, CO_2 reduction, and recently for electrochemical sensing, biomass catalysis and solar energy conversion. Now we implement and developing new methods for making advanced electro-functional nanomaterials and nanoclusters derived from thin-films molecular assemblies, inorganic nanomaterials and metal-oxides displaying great potential to be used in high performance water splitting catalysis and for chemical energy conversion and storage schemes. In this discussion we also highlight the challenges in chemical energy conversion and the possible way forward.

Emerging Technologies in Environmental Sciences: A Paradigm Shift for Sustainable Solutions

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Abstract:

The environmental sciences are undergoing a profound transformation as new technologies converge to address pressing ecological and sustainability challenges. This plenary lecture will explore a broad array of emerging technologies driving this change, including the use of artificial intelligence (AI) and machine learning (ML) to enhance climate modeling, biodiversity monitoring, and the development of early-warning systems for environmental risks. Furthermore, remote sensing technologies, including satellite and drone applications, are providing unparalleled accuracy in tracking land-use changes, deforestation, and pollution, supporting data-driven conservation and resource management. In addition to technological advances, nature-based solutions are increasingly utilized to restore and maintain environmental health. Phytoremediation, the use of plants to treat waste and contaminated soils, represents a key innovation in eco-friendly waste management. Birds and fungi are also being recognized for their role in environmental restoration: certain bird species support ecosystem balance through seed dispersal and pest control, while fungi contribute to bioremediation by breaking down pollutants in soil and water. Coupled with sensor networks and IoT technology, which allow real-time monitoring of air, water, and soil quality, these nature-based solutions exemplify a holistic approach to environmental management. Advances in genomics and biotechnology further enhance our ability to address ecosystem degradation, supporting efforts in biodiversity conservation, ecosystem restoration, and carbon capture. Additionally, blockchain technology offers transparent, traceable systems for environmental monitoring, supporting regulatory compliance and fostering sustainable resource use across industries. This lecture will discuss these technologies' potential to drive sustainable change, highlighting global case studies where they impact ecological restoration, resource efficiency, and climate resilience. Integrating these novel tools and biological approaches offers a transformative path for environmental stewardship in a rapidly changing world.

Perfluoroalkyl Acids: Emerging Pollutants in the Environment

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Abstract:

Perfluoroalkyl acids (PFAAs) are categorized as emerging contaminants because the information about their persistence, omnipresence, and toxic effects has been available only since the last 15 years due to continuous improvement of liquid chromatography-tandem mass spectrometry that can quantify these persistent organic pollutants in various matrices at trace levels. However, it would be better if another method could crosscheck LC measurements to avoid uncertainties due to background contamination. Therefore, in the present study, gas chromatography-mass spectrometry (GC–MS) and LC–MS 2 methods were developed to determine PFAAs in aqueous samples. GC method was less appealing than the LC method because of higher detection limits, a small range of analytes, and laborious derivatization before chromatographic separation. However, both GC–MS and LC–MS 2 methods had comparable performance characteristics and could be used to produce valid results. Continuous monitoring of the aquatic environment is vital for controlling and managing the transport of PFAAs and associated risks to human health and the environment. One part of this work, therefore, described the sampling and analysis of water and sediment samples collected from different locations (mainly from the river Saale, and additionally a few samples from the Elbe, Pleiße, Weiße Elster flowing through Germany, and from the river Sosiani of Kenya). Annual discharge of PFAAs from the river Saale into the Elbe was 164±23 or 91±39 kg y –1 when estimated from the analysis of grab samples or the POCIS (polar organic chemical integrative sampler) deployed for 20 days, respectively. Perfluorooctanoic acid (PFOA), a potential carcinogen, was the most abundant PFAA in most of the aqueous samples, whereas the prohibited perfluorooctane sulfonate (PFOS) was only found in some samples at low concentrations. In sediment samples from the river Saale, most short-chain PFAAs (≤ C6) were observed near/below their respective detection limits and could not be

quantified. Total loads of sediments were in the range of 1.9–4.2 ng g −1 , dominated by the long-chain PFAAs, and the most abundant PFAA in sediment samples was perfluorododecanoic acid (PFDoDA).

Enzyme-free Isothermal Amplification Dual-Target DNA Biosensors for Early Metastatic Breast Cancer Diagnosis

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Abstract:

Early diagnosis of metastatic breast cancer (MBC) plays a pivotal role in improving patient survival rates and optimizing treatment outcomes. Among more reliable and accessible molecular diagnostic tools that can detect metastatic markers in the early stages of cancer progression, DNA biosensors have emerged as promising platforms for the rapid, sensitive and cost-effective detection of cancer biomarkers. In this regard, we have developed one of the most innovative approaches, that is, enzyme-free isothermal amplification (catalytic hairpin assembly-CHA) combined with dual-target DNA biosensing. The CHA offers several advantages over traditional PCR-based methods, including faster reaction times, simpler instrumentation and higher specificity which make them ideal for point-of-care diagnostics and for developing user-friendly, portable biosensor devices. The dual-target approach allows for the simultaneous identification of multiple genetic markers, providing a more comprehensive understanding of the cancer's molecular landscape. This sharing of information will highlight the potential of DNA biosensors in transforming the landscape of cancer diagnostics and paving the way for more effective, accessible, and affordable healthcare solutions.

Photocatalytic Activity of Bi Doped CuO-rGO Nanocomposite for Removal of Crystal Violet Dye

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Abstract:

Graphene has gained attention as a truly two-dimensional material due to exceptional physicochemical qualities like large surface area, superior conductivity, outstanding mechanical properties, and simplicity of functioning and massive production. As it is produced at an affordable price, can be processed using a solution, and is versatile. rGO has been considered an ideal substitute for pristine graphene. Among the most exciting developments for massive and cheap manufacture of graphene-based products is graphene preparation via chemical reduction of graphene oxide (GO). The sustainable production of reduced graphene oxide (rGO) is critical for the creation of carbon nanotechnology. This study presents a green and environment friendly technique for the synthesis of rGO using lemon leaves extract as the reducing agent. Then nano composite is doped by bismuth. Both the doped and undoped nano composites were characterized by various techniques like SEM, FTIR, XRD and UV-Visible spectroscopy. The UV visible spectra of Graphene oxide indicated the peak at 225nm and for the reduced graphene oxide, the peak was observed at 260nm. The UV visible peak for the CuO-rGO composite was observed at 270nm and for the Bi doped CuO-rGO nano composite, UV visible spectra shows the peak at 275nm. The FTIR spectra of the undoped CuO-rGO shows the peak at 702cm^{-1} and the FTIR spectra of the bismuth doped sample indicated a peak at 734cm^{-1}. The crystallite size calculated by Scherrer equation is 6nm for the undoped composite. The crystallite size was 9nm for the doped composite. Both the doped and undoped nano composites were used for dye degradation and effect of various parameters were also studied and optimized. The maximum removal of the dye for the undoped composite was 97.2% when exposed for 100min. While the doped showed 99.8% removal within 40min. The bismuth doped CuO/rGO nano composites showed high photo catalytic activity than undoped composite.

Electro-Oxidation of Strontium Tungstate Fabricated Graphitic Carbon Nitride for Hydrogen Production via Water Splitting

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Abstract:

One sustainable way to get around the issues with fossil fuels is to use a clean energy source to produce hydrogen by electrocatalytic water splitting. The development of a non-precious, stable, and extremely effective electrocatalyst is therefore crucial. The well-known carbon material, graphitic carbon nitride has several uses and excellent physical and chemical characteristics, which make it an interesting option for electrocatalytic sensing. Graphitic carbon nitride was used in this study for manufacturing metal tungstate nanocomposites by the hydrothermal process and strontium was used as a precursor. FTIR and XRD were used to characterize the g-C3N4/SrWO4. The FTIR spectra verified the existence of a functional group between the metal and tungstate groups. While the vibrational absorption bands for metals emerge in the 400–600 cm-1 range, the nanocomposites exhibit a tungstate peak at 600 cm-1 . X-ray diffraction (XRD) analysis confirmed the successful formation of all nanocomposites, with distinctive peaks matching the JCPDS standard and an average particle size is 84.4 nm. Cyclic voltammetry is used to perform electrochemical water splitting in alkaline media to investigate the active surface area of the synthesized g-C_3N_4-$SrWO_4$ modified electrode, which is 0.081 cm^2. Cyclic voltammetry (CV) curves were recorded in a 1M KOH supporting electrolyte solution at various scan rates (10 mV/s to 100 mV/s) for the g-C_3N_4-$SrWO_4$ modified electrode, with a diffusion coefficient of 132.06 × 10^{-6} cm^2/s. The synthesized nanocomposite had improved conductivity qualities and an effective catalyst for water splitting.

Electro-Oxidation of Stannous Tungstate Fabricated Graphitic Carbon Nitride for Hydrogen Production via Water Splitting

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Abstract:

Hydrogen is a highly efficient, clean energy source due to its lack of carbon emissions, but effective catalysts are necessary for its production through electrochemical water splitting. Graphitic carbon nitride (g-C3N4) a well-known carbon material, has a lot of potential for electrocatalytic sensing because of its diverse functions and superior physicochemical characteristics. This study synthesized Stannous-tungstate nanocomposites derived from g-C3N4 using a hydrothermal method to explore their potential in hydrogen production. Stannous served as a precursor in synthesizing the g-C3N4-SnWO4 nanocomposite, which was characterized using FTIR and XRD. FTIR analysis confirmed functional groups linking stannous and tungstate, showing metal absorption bands in the 400–600 cm^{-1} range and a tungstate peak at 600 cm^{-1}. XRD results aligned with known JCPDS patterns, verifying the nanocomposites successful formation having average particle size of 9nm. Cyclic voltammetry is used to perform electrochemical water splitting in alkaline media to investigate the active surface area of the synthesized g-C_3N_4-$SnWO_4$ modified electrode, which is 0.061 cm^2. Cyclic voltammetry (CV) curves were recorded in a 1 M KOH supporting electrolyte solution at various scan rates (10 mV/s to 100 mV/s) for the g-C_3N_4-$SrWO_4$ modified electrode, with a diffusion coefficient of 40.72×10^{-6} cm^2/s. The nanocomposite exhibited improved conductivity and served as an effective catalyst for water oxidation, indicating its potential use as an electrode material for direct hydrogen evolution in clean energy production.

Study of Polyacrylamide Mediated Peanut Shell/Alumina Ternary Composite for Removal of Dyes from Water

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Abstract:

Dyes are one of the most common water pollutants, and they are associated with a variety of biological and environmental issues that have negative consequences. Recent research focusses on using an affordable adsorbent to mitigate toxic dye pollution from aqueous solutions. In order to examine the removal efficiency of direct orange-26 (76.2%) from the aqueous solution, alumina supported by peanut shells was made using a co-precipitation method and polyacrylamide. The produced composite was assessed using FTIR, SEM, and XRD methods. The adsorption of dye is significantly influenced by the presence of -OH, -COOH, and -NH2 groups. In order to achieve effective dye removal, batch adsorption experiments were conducted by adjusting various parameters, including pH, contact time, adsorbent dose, and initial dye concentration. The ideal pH, adsorbent dose, initial dye concentration, and contact time were 0.05g, 50mgL^{-1} and 4 hours, respectively, for the highest dye removal (78.63%) and sorption capacity (39.31 mgg-1). The pseudo-second order and Langmuir isotherm models provided a clear definition of the sorption data. Accordingly, the findings demonstrated that the peanut shell composite mediated by polyacrylamide is a viable material for treating textile effluents and is highly effective at removing direct orange-26 from the aqueous solution.

Removal of Dyes by Bimetallic Nanoparticles incorporated onto Metal Organic Framework: A Sustainable Approach

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Abstract:

Growing pollution from industrial wastewater necessitates creative, environmentally friendly solutions to protect the environment and public health. Through the green synthesis of Cu/Zn bimetallic integrated into MOF-5(Metal Organic Framework), this study presents a unique, environmentally friendly method of wastewater cleanup. Superior photocatalytic activity is demonstrated by the Cu/Zn-MOF-5 hybrid, which uses Monoon longifolium (False ashoka) as a renewable precursor. photocatalysis is becoming a very appealing, cost-effective, as well as eco-friendly environmental remediation technology as compared to other conventional methods. Therefore, creating stable and efficient photocatalysts is crucial. Peaks at 285 nm, 300 nm, and 315 nm were detected by UV-visible spectroscopy, demonstrated that the green synthesis of Cu/Zn@MOF-5, bimetallic (Cu/Zn oxide) nanoparticles, and plant extract. The material's crystallinity, crystallite dimension, and 11.9 nm particle size were all validated by characterization methods (FT-IR, SEM, XRD, EDX and ZETA). FTIR confirmed that the CuO and Zn-O bond were found at 530cm-1 and 550cm-1. The peak at the range of 1335-1420cm1 showed the presence of CH group that was present in the terephthalic acid. The photocatalytic process was adjusted using response surface approach, which revealed the optimal parameters: pH 3 for methyl orange and pH 10 for crystal violet, 5 mg catalyst dosage, 120 min irradiation time, and 20 ppm starting concentration. Under ideal circumstances, the Cu/Zn-MOF-5 hybrid showed exceptional photocatalytic efficiency by decolorizing methyl orange by 92% and crystal violet by 87% when exposed to UV light. This study synthesized a newly developed nano-Cu/Zn bimetallic incorporated onto MOF-5 with exceptional photocatalytic activity utilizing a green technique with Monoon longifolium.

Synthesis and Application of Rice Husk Derived Cellulose Composite with Graphene Oxide as Potentially Effective Adsorbent for Dyes Removal

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Abstract:

Dyes in wastewater are environmentally toxic and should be removed from water bodies. For this purpose, adsorption technique which is low cost and effective among all the possible dye removal methods was used to remove synthetic dyes i.e., Rhodamine-B (Rh-B), Methylene Blue (MB) and Methylene Violet (MV). Agricultural wastes i.e. rice husk (RH) was used to extract cellulose which were further used to synthesize composite with Graphene oxide i.e., Cellulose-Graphene oxide (C-GO) to enhance the adsorption capacity for dye removal. Characterization of the composite was done by FTIR, SEM, EDX, XRD and TGA. Maximum removal of selected dye was optimized by adsorption controlling parameters e.g. Influences of initial dye concentration (10-100ppm), temperature=30-60^{o}C, solution pH=2-11 and contact time 20-110min. Results revealed that maximum adsorption capacity 92mg/g was achieved against Rh-B. Adsorption thermodynamics, equilibrium and kinetic study were performed. Thermodynamics study revealed that it was exothermic and spontaneous reaction with all the three dyes. Equilibrium results showed that Langmuir, Freundlich and Temkin were best fitted with Rh-B, MV and MB respectively. Pseudo-second order kinetic was best fitted with the three dyes. On the basis of results composite has shown promising results with Rh-B dye.

MXenes based Nanostructures for Electrochemical Sensing

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Abstract:

MXenes (M n+1 X n T x), a class of transition metal carbides, nitrides and carbonitrides, exhibit distinct physical and chemical characteristics as 2D nanomaterials. MXenes feature high electrical conductivity, hydrophilicity, unique layered topology. Owing to these characteristics, MXenes-based materials find significant applications in electronics, energy storage devices, catalysis, sensing for biomedical and environmental applications. MOFs present a class of highly porous materials with large specific surface area, tunable structure, and active transition metal redox centers, making them highly suitable for electrochemical sensing. Reliable and sensitive detection of Bisphenol-A (BPA) i.e. a well-known endocrine disruptor has become one of the most persuasive environmental concerns vis-à-vis consequences of micro plastics on living organism. The synergistic interaction between MXenes and MOFs provide a potential platform for the recognition of such water borne endocrine disruptors. Larger surface area and terminal functionalities of these materials facilitate the direct electron transfer of the beset analyte in electrochemical sensing with enhanced signal response, high sensitivity and low detection limit.

Synthesis of N-Alkyl Azoles Carrying Cerium Complexes and Cerium Oxide Nanoparticles for Catalytic and Medicinal Applications

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Abstract:

The alarming rise in water pollution caused by industrial effluents, especially dyeing reagents, poses significant threats to aquatic ecosystems and human health. Simultaneously, the growing resistance of cancerous cell lines to existing anticancer drugs exacerbates health challenges. This study presents the synthesis of N-alkylated imidazole derivatives and their cerium complexes: tetrakis(3-propyl-2,3-dihydro-1H-imidazol-1-yl)cerium(III) nitrate (C1) and tetrakis(3-butyl-2,3-dihydro-1H-imidazol-1-yl)cerium(III) nitrate (C2), along with cerium oxide nanoparticles. Structural and chemical characterizations of the synthesized compounds were performed using FT-IR, FT-Raman, and NMR spectroscopic techniques. The catalytic potential of the synthesized cerium complexes was evaluated for the degradation of hazardous dyes such as Methyl Orange (MO) and Murexide (MX). Using Response Surface Methodology (RSM) with a Central Composite Design (CCD) model, key variables like contact time, catalyst dose, and concentration were optimized, achieving impressive degradation efficiencies of 80– 90 %. Additionally, the pharmacological properties of the synthesized ligands and complexes were investigated for their ability to inhibit the growth of cancerous PC3 (prostate cancer) and HeLa (cervical cancer) cell lines. IC50 values ranged between 21–23 µM for PC3 cells and 12.72–19.51 µM for HeLa cells, demonstrating competitive efficacy compared to the reference drug Doxorubicin. The multifunctional properties of these cerium-based compounds, spanning catalytic and medicinal applications, address critical environmental and health challenges, making them promising candidates for sustainable chemistry and pharmaceutical advancement

Nanoparticle-Induced Systemic Resistance in Mungbean against Yellow Mosaic Virus

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Abstract:

Silver nanoparticles (AgNPs) have emerged as a promising tool for managing plant viral diseases due to their potent antiviral properties. This study aimed to evaluate the effectiveness of AgNPs as foliar curative agents against Yellow Mosaic Virus (YMV) in mungbean (*Vigna radiata*). AgNPs were applied 24 hours post-virus inoculation to assess their viricidal activity. The results demonstrated that AgNPs effectively inactivated YMV, with a significant reduction in disease presence. A concentration as low as 100 mL per liter of AgNPs was sufficient to prevent disease symptoms, while complete inhibition of viral infection was observed at 200 mL per liter. AgNPs displayed high bioreactivity, binding to viral particles and suppressing their replication and accumulation within plant tissues. Furthermore, AgNP treatment induced systemic resistance in mungbean plants by upregulating the expression of pathogenesis-related protein (PR-1) and enhancing the production of defense-related oxidative enzymes. Ten days post-treatment, viral infection was reduced by 25% and 60% at AgNP concentrations of 250 mg/L and 300 mg/L, respectively. These findings suggest that AgNPs possess curative viricidal activity by targeting the viral coat proteins, thereby inhibiting virus replication. The study highlights the potential of AgNPs as an eco-friendly strategy to control viral diseases and mitigate virus transmission in mungbean cultivation under field condition

Nanotechnology for Sustainability: Bridging Innovation and the SDGs

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Abstract:

Nanotechnology, the science of the extraordinarily small, is creating monumental impacts on sustainability. Engineering materials at the nanoscale unlock groundbreaking solutions that address humanity's most pressing challenges, seamlessly intertwining innovation with the Sustainable Development Goals (SDGs). In the quest for clean energy (SDG 7), nanomaterials power ultra-efficient solar cells, revolutionize batteries and enable hydrogen fuel technologies. For water security (SDG 6), nanotechnology introduces advanced filtration systems that transform polluted or saline water into drinkable sources, ensuring access to clean water even in arid regions. In healthcare (SDG 3), nanomedicine enables precision drug delivery, shrinking treatments to the size of cells while combating drug-resistant pathogens with nano-antimicrobial surfaces. Agriculture (SDG 2) benefits from nano-fertilizers and nano-pesticides that boost productivity while reducing environmental harm, ushering in a new era of sustainable food production. However, the journey isn't without challenges. Ethical dilemmas, potential environmental risks, and disparities in global access demand careful navigation. With robust governance and interdisciplinary collaboration, nanotechnology's promise can flourish responsibly. By fusing science with purpose, nanotechnology emerges as a cornerstone of sustainability, redefining progress for future generations. Its potential inspires a vision where technological innovation and environmental stewardship walk hand in hand.

Benign-by-Design Preparation of Nanomaterials for Catalytic and Sustainable Applications

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Abstract:

The synthesis of environmentally benign materials is a key aspect of green chemistry. Interconnected porous materials offer significant potential in this field due to their high surface-to-volume ratio, tunable pore sizes, and customizable physicochemical properties. These materials are not only eco-friendly and cost-effective but also adhere to the 3 Rs (reduce, reuse, recycle). They are synthesized using bottom-up and top-down approaches, which reduce the use of toxic chemicals. Their versatile shapes and efficient mass transport capabilities make them ideal for applications in homogeneous and heterogeneous catalysis, enhancing reaction efficiency. Additionally, their large surface area and reactive sites accelerate reactions, minimizing chemical use, and improving photocatalytic performance for pollutant degradation. The integration of these materials into sustainable development aids in addressing environmental pollution, the energy crisis, and achieving sustainable development goals.

Collaboration of Material Science and Conventional Instrumental Analysis for Sensitive Analysis of Drug Molecules

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Abstract:

Sensitive analysis of organic molecules in biological samples is a big challenge for analytical chemists. One of the most studied target organic molecules in biological samples are drugs which is so important for drug development studies, pharmacokinetic analysis, toxicological evaluations, and diagnosis tests need millions of clinical analyses every day. There are two challenges in analysis of biological samples for any kind of molecule or ion. The first one is the intensive and complex structure of the sample matrix. These type samples include a lot of interfering compounds, big biomolecules, and active biological content. The second one is generally a very low concentration of target molecules compared with matrix components. It is required to carry out this analysis. Unfortunately, most conventional research laboratories don't have this possibility. Use of various sample pre-treatment procedures facilities these analysis by means of increasing analytical signals and removing matrix component. This is provided by collaborations between material sciences and chemical analysis. Sensitive analyses are possible by conventional instrumental system if a sample pre-treatment procedure was applied before determination step. The main aim of this procedure is separation of matrix compounds and pre-concentration of target molecules. So, the detection system can easily determine target concentrations. Most used sample pre-treatment procedures are solid phase extraction (SPE)-based methods. Use of natural and synthetical materials in SPE systems increases the sensitivity of analysis and accuracy in trace analysis.

Economics of Panoramic Drug Discovery of Natural Products

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Abstract:

Natural product chemistry plays a pivotal role in every sphere of our life, including health care and as well as agriculture. The substantial contribution of natural product chemistry is commendable. There has been a renewed interest in natural product research as the other methods of alternative drug discovery have been failed to deliver many lead compounds in key therapeutic areas. Therefore, it is indispensable to continue to be competitive with other drug discovery methods with improved natural product research needs for the screening, isolation, and structure elucidation processes, as well addressing the issues involved with large-scale compounds supply. Present work deals with several on-going research discoveries in our lab from discovery of micromolecules to macromolecules to find potential cure for the diabetes, cancer, and urolithiasis. Moreover, some green insecticides, fungicides and herbicides were also discovered from plants. Therefore, the use of bio-based pesticides is essential for green environment in changing scenario of climate change. The work also contains some greener methods of biotransformation of drug molecules and determination of their enhanced activities through molecular docking and ADME analyses.

Functional Nanomaterials – Tuning the Size and Surface Chemistry for Applications in Biomedical Science, Renewable Energy Technologies and Environmental Remediation

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Abstract:

The unique chemical and physical properties of nanoscale materials have triggered great scientific interest to explore their potential applications in biomedical sciences, renewable energy technologies, environment, catalysis, and industry etc. The chemical and physical properties of metal/ metal oxide nanoparticles can generally be tuned by controlling their size, shape, and surface chemistry. In this regard, we have developed several reproducible protocols based on chemical reduction and precipitation approach to prepare functionalized metal/metal oxide nanoparticles from sub-nanometer to over 100nm in aqueous/organic media with a decent control over their size, shape, and surface chemistry. Many of these metal nanoparticles have been used as building blocks to design/synthesize new nanostructured materials with tunable nanoscale features using template-based and template-less strategies. The functionalized metal/metal oxide nanoparticles/nanoclusters possess interesting optical, recognition and catalytic/bio-catalytic properties, and currently we are focusing on the applications of the functionalized nanoparticles and nanocomposites in biomedical sciences (i.e., bio-sensing especially bacterial detection, bio-imaging, drug delivery and multidrug resistance etc.), environmental remediation (detection and removal of organic/inorganic pollutants from water, CO oxidation, and CO_2 capture and conversion) and renewable energy technologies (mainly H_2 production & storage and electrode materials for batteries) based on electrocatalytic and photocatalytic approaches. This talk would, therefore, be an overview of interdisciplinary research activities of Functional Nanomaterials Group at LUMS to synthesize customized inorganic/organic nanoparticles with tunable size and surface chemistry, and their composites having unique chemical and physical properties, and subsequent applications in biomedical sciences, environment, catalysis and renewable energy technologies.

Green Extraction Techniques for Clean Label Recovery of Polyphenols from Plant Sources

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Abstract:

Phytochemicals called polyphenols are naturally prevalent in plant matrices. The various health advantages and therapeutic effects of polyphenols have recently attracted the attention of researchers worldwide. These effects aim to promote overall health and wellness by mitigating oxidative stress and lifestyle-related illnesses. For ages, traditional extraction techniques havekhy been used to extract polyphenols. These traditional techniques have a number of built-in drawbacks, and finding a single, standardized, and optimal technique to extract polyphenols efficiently, quickly, and cleanly has proven to be a difficult undertaking thus far. Using a more environmentally responsible approach, the commercial use of phenolic compounds as natural antioxidants and supplements has increased research into economical, effective, and environmentally friendly extraction techniques. The advantages, disadvantages, factors governing extraction mechanisms, and applications of modern extraction techniques, including pressurized liquid extraction, pressurized hot water extraction, ultrasound-assisted extraction, microwave-assisted extraction, and supercritical fluid extraction, as green alternatives to conventional extraction methods, were presented in this overview along with updated technical information. The focus was on clean-label extraction of phenolic compounds from plant matrices. Furthermore, by addressing the drawbacks of traditional methods for polyphenol extraction, new extraction techniques offer significant advantages such as reduced solvent and time consumption with much lower operational costs. In order to extract polyphenols from plant matrices and their byproducts on an industrial scale, more study is required to examine the principles underlying the extraction kinetics of green extraction techniques.

Emerging Trends in the Extraction of Bioactive Ingredients from Selected Fruits, Oil Seed and Agrowastes

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Abstract:

Extraction of high-value components from various plant materials is always a challenging task. Currently, there is growing interest in the use of cutting-edge green extraction techniques that can produce healthy extracts for the development of functional foods and nutra-pharmaceuticals. In this lecture, we explored effective recovery of phenolics, lipids and essential oils from selected food plants and agro-waste through the use of optimized green extraction methods such as ultrasound-assisted extraction (UAE), enzyme-assisted extraction (EAE) and enzyme-assisted supercritical fluid extraction (EA-SFE). The recovered bioactive components have been analytically characterized using advanced chromatographic approaches such as GC-MS and LC-MS. Overall, significant improvement in the nutraceutical prospects of the extracted components was examined as compared with control. Optimized UAE and EA-SFE were found to be effective for recovering phenolics from olives, jujube fruit, pomegranate peel, and black tea residue, where applicable. EAE and SFE were highly successful towards improving the antioxidant attributes of isolated sesame and hemp seed oils, as well as basil and Eucalyptus essential oils. While, response surface methodology and artificial neural networking-based optimized EAE produced the best yield of phenolics from balsam apple, mulberry leaves and Capparis fruits. Significant alterations in the ultrastructure of the residual materials were observed by field-emission scanning electron microscopy (FE-SEM), confirming that these pre-treatments successfully broke down and hydrolysed the cell walls, allowing the improved recovery of bioactives. These techniques can be employed to improve the extraction of nutraceutical components from a range of fruits, oliseeds and agro-wastes.

Antidiabetic Activity based Fortification of Olive and Mustard Oils using *Mangifera indica* (Mango), *Azadirachta indica* (Neem) and *Fagonia indica* Plant Extracts

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Abstract:

Diabetes mellitus, a chronic metabolic condition that eventually causes serious harms to the kidneys, nerves, heart and blood vessels, is characterized by high levels of blood glucose. Mustard and olive oil will be blended with extracts of *Mangifera indica*, *Azadirachta indica*, and *Fagonia indica* followed by their biological screening and characterization. Plant extracts may offer additional therapeutic, such as hepatoprotective, antiinflammatory, antibacterial, analgesic, and antioxidant qualities. Emulsions will be formed using several methods with the help of different emulsifiers. Emulsions improve the properties of vegetable oils by increasing specific surface area by reducing droplet size. These emulsions will be assessed for their antibacterial, antioxidant, and antidiabetic properties. There will be individual phenolic analysis by HPLC, total phenolic analysis, flavonoid analysis, and volatile component analysis by spectroscopic methods. The experiment will be conducted using three replications and six treatments. One-way analysis of variance (ANOVA) will be used for analysis purpose whereas means will be compared using Tuckey test.

Effects of Polyphenol-Rich *Hibiscus* and *Zingiber* Teas on Obesity and Oxidative Stress in Rats Fed a High-Fat-Sugar Diet

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Abstract:

The present research work was planned to investigate the potential of polyphenol rich extracts of *Hibiscus rosa-sinensis* (HRS) and *Zingiber officinalis* (ZO) teas against the obesity and related biochemical parameters of high-fat-sugar diet-induced obesity rats. Three herbal teas were prepared from HRS flowers and ZO rhizomes and their mixture (HRS:ZO, 3:1). Extracts were prepared and total reduced capacity (TRC) and total flavonoid contents (TFC) of the extracts were estimated as gallic acid and catechin equivalents (GAE and CE), respectively. TRC of HRS and ZO extracts were found to be 5.82 and 1.45 mg/g of dry plant material, measured as GAE while TFC were 9.17 and 1.95 mg/g of dry plant material, as CE, respectively. Reverse Phase-HPLC analysis revealed the presence of 15 phenolic acids and 4 flavonoids in herbal extracts of both samples. Catechin, rutin, gallic acid, 4-hydroxy benzoic acid, chlorogenic acid, caffeic acid and salicylic acid were the major compounds detected. 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging assay was performed and both extracts showed > 50% DPPH radical scavenging capacity. Two levels (250 and 500 mg/kg BW) of each tea were selected to assess anti-obesity potential using high-fat-sugar-diet-induced obesity rat's model. Data showed that higher dose of HRS significantly reduced the rat's body weight and body mass index as compared to high-fat-sugar diet group. Total cholesterol, high- and low-density lipoproteins, triglycerides, kidney, liver and atherogenic indexes, bilirubin total, aspartate aminotransferase, alanine aminotransferase, alkaline phosphate and serum creatinine of rats showed that HRS extract showed significant anti-obesity potential. Moreover, HRS extract also prevent the alterations in malondialdehyde, superoxide dismutase and reduced glutathione levels of experimental rats, thus also showed potential against oxidative stress. It is evident from the results that higher dose of HRS exhibited best protective effects against obesity and oxidative stress while ZO showed fewer protective effects.

Exploration of Antidiabetic and Antioxidant Potentials of *Morus* Leaves

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Abstract:

Diabetes is a metabolic disorder that causes high blood sugar due to poor insulin production. Prolonged elevated blood sugar levels have the potential to harm the kidneys, nerves, and blood vessels. Diabetes was treated with insulin and drugs, but extended use of some drugs may lead to side effects and drug resistance. Plant based medications are in high demand these days to treat a variety of disorders due to their fewer negative effects when compared to manufactured counterparts. The purpose of this thesis was to examine the possibility of enhancing the anti-diabetic and antioxidant effects of Morus (mulberry) leaves. Morus leaves have been used to treat diabetes and infectious diseases. The flavonoids obtained from these leaves have favorable hypoglycemic effects. 1-Deoxynojirimycin (DNJ) in mulberry leaves helps to regulate Glucose levels in the blood of individuals with diabetes. Leaves extraction was done in ethanol, methanol and acetone. The DPPH test was utilized to measure antioxidant activity, and the α-amylase assay was employed to assess antidiabetic activity. Using the disc diffusion approach, antimicrobial activity was achieved by preventing the development of microorganisms. Each result was presented as mean ± standard deviation and subjected to one-way ANOVA statistical analysis, utilizing Tuckey's Test for comparisons. According to the study, methanol extract of black mulberry leaves had marginally stronger antioxidant and antidiabetic properties than ones made extract with other solvents. Thus, methanol was the most effective solvent for extracting antioxidants, such as rutin, chlorogenic acid, and isoquercitrin, from mulberry leaves.

Development of Multifunctional Bioactive Food Packaging based on Silver Nanoparticles/Grape Fruit Peel Extract Reinforced PVA Composites

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Abstract:

Active food packaging based on bio-wastes has gained considerable attention these days due to their ecofriendly and biodegradable behavior. In this study, multifunctional bio-composite films with remarkable anti-oxidant and anti-microbial attributes were synthesized by incorporating biosynthesized silver nanoparticles (AgNPs) and grape fruit peel extract (GFPE) into polyvinyl alcohol (PVA) matrix. Synthesized films were characterized in terms of Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), Scanning electron microscopy (SEM), Differential scanning calorimetry (DSC) and Dynamic Mechanical Analyzer (DMA). Antioxidant activity of AgNPs-GFPE/PVA films was determined by %DPPH scavenging ability and Ferric reducing antioxidant power assay while antimicrobial activity was measured by agar diffusion method. XRD analysis revealed the semicrystalline behavior of synthesized composites with characteristics peak at 38◦ whereas SEM micrographs confirmed the homogeneous dispersion of reinforcement and porous rough surface structure of AgNPs-GFPE/ PVA nano-composites. AgNPs-GFPE/PVA nanocomposite exhibited glass transition temperature (Tg) at ~116 ◦C and Tm ~191 ◦C along with the storage modulus of 685 MPa, revealing significantly enhanced thermal and mechanical stability of composites compared to pure PVA films. The composite films exhibited remarkable antioxidant potential i.e DPPH scavenging activity ~50 % and reducing power ~ 0.58. The AgNPs-GFPE/PVA nano-composite films exhibited remarkable antimicrobial activity in response to food borne pathogens. The results designated that the synthesized composite films have prodigious potential of being cheap, eco-friendlier substitute to conventional materials for application in food packaging, which certify the safety and economical life span of packed food.

Facile Fabrication of Novel Silver-Polypyrrole-Multiwall Carbon Nanotubes Nanocomposite for Replacement of Platinum in Dye-Sensitized Solar Cell

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Abstract:

In this work, high performance silver-polypyrrole multiwall carbon nanotubes (Ag-PPy-FMWCNTS) nanocomposites are easily synthesized using the electrodeposition technique on a stainless steel substrate, and they are used as an inexpensive counter electrode (CE) for the precious metals free of platinum (Pt) DSSC. Numerous methods, including Fourier transform infrared (FTIR), X-ray diffraction, scanning electron microscopy (SEM), cyclic voltammetry (CV), and the four probe technique, were used to analyze the nanocomposites. The Ag-PPy-FMWCNTS nanocomposites CE exhibit good electrocatalytic activity and low charge transfer resistance Rct (2.50 Ω cm2) for I3-/I- redox solution, according to cyclic voltammetry and Tafel polymerization tests. The Ag-PPy-FMWCNTS nanocomposite's high electrical conductivity (226S cm-1) was demonstrated by the four probe investigations. The DSSC with Ag-PPyFMWCNTS nanocomposites CE has a respectable solar to electrical conversion efficiency of 7.1%, which is greater than the efficiency of the DSSC with a thermally dissolved Pt reference electrode of 7.6%, and a notable short circuit current density of 13.95 mAcm-2. The outstanding Ag-PPy-FMWCNTS nanocomposites' conversion efficiency, quick charge transfer, cheap cost, and straightforward fabrication process make them a viable and effective alternative to Pt CE for the large-scale manufacturing of DSSC.

Synthesis of Modified Tio$_2$ Nanoparticles for the Development of Multifunctional Substrate

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Abstract:

For sustainable approach in nanotechnology application, the resource-intensive process was modified with lessen ecological impact. The conventional application of nanoparticles on substrate requires multiple complex steps which is time and energy consuming and also require specialized equipment leading towards limitations of accepting challenges to meet rapid technological and ecological demands. This study elaborates the procedure of in-situ synthesis and application of TiO_2 modified nanoparticles using sol-gel method. TiO_2 nanoparticles were synthesized using titanium tetraisopropoxide as precursor along with octadecyltrimethoxysilane and glycidoxypropyl trimethoxysilane as modifying agent. This chemical finish can directly be used to decorate the substrate without any extra application process thus minimizing the ecological impact. The resulting nanoparticles were characterized using SEM, EDX, FTIR, XRD, and DLS (zeta sizer) analysis. XRD confirmed the formation of the anatase phase with a particle size of 17.9 nm, while a zeta potential of -23.3 mV indicated excellent dispersion stability. These particles were directly applied to a cellulosic substrate, avoiding intermediate processing steps. FTIR analysis revealed strong bonding between the modified nanoparticles and the substrate, enhancing adhesion. Surface roughness changes were evaluated using the Kawabata Evaluation System, demonstrating minimal impact on the substrate's integrity. Furthermore, UV protection and antibacterial properties were evaluated showing promising result with excellent adherence. Hydrophobic properties were assessed via water-contact angle, reaching 157.9°, indicating superhydrophobic character. The successful development of multifunctional fabric with modified nanoparticles containing excellent durability affirms the approach towards sustainability.

Unveiling the Solubilization Behavior of Nickel, Cobalt and Zinc Fluoride Complexes in Micellar Media of Sodium Lauryl Sulphate by Conductometery, UV/Vis and ^{1}H-NMR Spectroscopy

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Abstract:

For sustainable approach in nanotechnology application, the resource-intensive process was modified with lessen ecological impact. The conventional application of nanoparticles on substrate requires multiple complex steps which is time and energy consuming and also require specialized equipment leading towards limitations of accepting challenges to meet rapid technological and ecological demands. This study elaborates the procedure of in-situ synthesis and application of TiO_2 modified nanoparticles using sol-gel method. TiO_2 nanoparticles were synthesized using titanium tetraisopropoxide as precursor along with octadecyltrimethoxysilane and glycidoxypropyl trimethoxysilane as modifying agent. This chemical finish can directly be used to decorate the substrate without any extra application process thus minimizing the ecological impact. The resulting nanoparticles were characterized using SEM, EDX, FTIR, XRD, and DLS (zeta sizer) analysis. XRD confirmed the formation of the anatase phase with a particle size of 17.9 nm, while a zeta potential of -23.3 mV indicated excellent dispersion stability. These particles were directly applied to a cellulosic substrate, avoiding intermediate processing steps. FTIR analysis revealed strong bonding between the modified nanoparticles and the substrate, enhancing adhesion. Surface roughness changes were evaluated using the Kawabata Evaluation System, demonstrating minimal impact on the substrate's integrity. Furthermore, UV protection and antibacterial properties were evaluated showing promising result with excellent adherence. Hydrophobic properties were assessed via water-contact angle, reaching 157.9°, indicating superhydrophobic character. The successful development of multifunctional fabric with modified nanoparticles containing excellent durability affirms the approach towards sustainability.

^{1}H-NMR and DLS Study of Formulated Microemulsion System Emulsified with Non-ionic Surfactant

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Abstract:

Microemulsions are technologically complex fluids of prime importance. These are thermodynamically stable, possess transparency, isotropic properties and characteristic structure with droplet size 5-100 nm, which gives them large interfacial area. In pharmaceuticals microemulsions facilitate the solubilization of poorly water-soluble drugs, leading to improved bioavailability and controlled drug release. This research work was an attempt to summarise important aspects like definition, method of preparation and methods of analysis of Pregabalin (an antileptic drug used to treat neuropathic pain) incorporated o/w microemulsions. Microemulsion systems comprised of Linoleic acid (Oil phase), TX-100(surfactant), short chain alcohols (ethanol, propanol) as cosurfactant and phosphate buffer (aqueous phase) were prepared. Conventional techniques were used to explore the microemulsions' characteristics (pH, conductivity, surface tension, partition coefficient, viscosity). DLS (dynamic light scattering) study was carried out to determine the particle size, particle size distribution and stability over time. Microemulsions remained stable for 9-10 months. Further ^{1}H-NMR analyses performed to investigate the targeted site of interaction of dug which revealed the presence of drug in hydrophilic shell of micelles. Hence, it is suggested that formulated microemuslions are stable with high drug loading capacity and have prolonged shelf-life along with their capability to protect the drug by entrapping it.

MEXENES as Versatile Materials for Energy Applications

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Abstract:

MXenes, being a newborn 2D nanomaterial has drawn its attention because of revolutionary properties and commercial applications. This thesis comprises of etching of d-Ti_3C_2, d-Ti_3CN and d-Ti_3N, V2C, and Ti3CN MXene from parent MAX phase. These new composite materials ware prepared using Ni_3S_4, MoO_3, V_2O_5, TiO_2, and ionic liquid (1-Methyl-3-butyl imidazolium Bromide) using different method of synthesis (hydrothermal, sonochemical method). The phase development and surface morphology of these novel materials were systematically examined using a range of characterization techniques such as X-ray diffraction (XRD), Raman spectroscopy, FTIR (Fourier transform infrared spectroscopy) X-ray photoelectron spectroscopy (XPS), scanning tunneling electron microscopy (STEM), and scanning electron microscopy (SEM). The surface porosity and electrochemical properties were thoroughly studied using gas sorption and state of the art electrochemical techniques. MXene and its nanocomposites were tested for energy applications such as supercapacitors (SCs) and water splitting. N-Ti_3C_2@Ni_3S_4 showed electrochemical results with specific capacitance (C_s) of 1280 F g^{-1} at a current density of 1 A g^{-1}. d-Ti_3C_2/MoO_3@IL showed exceptional performances with C_s of 1680 F g^{-1} at 1 A g^{-1}. Ti_3C_2/MoO_3 electrode possessing 2D/1D structure exhibits outstanding C_s of 624 F g^{-1} at 1 A g^{-1}. Similarly, d-Ti_3CN delivered an excellent C_s of 260 F g^{-1} at 1 A g^{-1} current density. Moreover, a symmetric supercapacitor (SSC) device from N-Ti_3C_2@Ni_3S_4, d-Ti_3C_2/MoO_3@IL and d-Ti_3CN demonstrated excellent energy and power densities. Ti_3C_2/MoO_3 and d-Ti_3C_2/V_2O_5 showed excellent results for water splitting applications (HER, OER). The results proved that MXene based composites can act as an advanced electrode material for fabrication of portable electronic materials.

Upcycling of PET Waste into Interfacial Solar Steam Generators: Advancing and Challenges

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Abstract:

Plastics crisis stands as one of the most pressing challenges for both Earth and humanity today. Up to 6.4 billion tons of plastic garbage produced globally each year, of which 9% recovered, 12% incinerated, and 79% accumulated in the environment. Upcycling of low-cost poly(ethylene terephthalate) (PET) waste into metal-organic frameworks (MOFs) is a cost-effective solution to the environmental impact of plastic waste, including the widespread "White Pollution". PET-derived MOFs have shown great potential across various applications, such as energy conversion and storage, photocatalysis, and adsorption. In the session talk, we will explore the strategy for converting plastic waste into a solar-driven interfacial water evaporator, optimization of physico-chemical parameters to improve the thermal performance and light absorption capabilities of these materials. Interfacial water evaporation approach effectively address a range of common water contaminants, including volatile organic compounds (VOCs), synthetic dyes, heavy metal ions, and other pollutants. Other than the comprehensive overview of the design, performance, and effectiveness of this technology in pollutant removal the challenges that currently limit the practical implementation of interfacial water evaporation systems in real-world wastewater treatment scenarios, such as scalability, durability, and economic feasibility will be discussed. Finally, the perspectives on the future directions and advancements needed to overcome these obstacles for wider adoption of this promising technology in sustainable water management practices will be discussed.

Effect of Titanium Doping on Conductivity, Density of States and Conduction Mechanism in Zno Thin Film

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ABSTRACT

High quality, ~120 nm thin ZnO and Ti-doped ZnO (TZO) films were deposited on silicon substrates using magnetron co-sputtering technique. Surface roughness of the films was ~2 nm. Ti incorporation effect on the structure, morphology, conductivity, density of states (DOS) and conduction mechanism was investigated in detail. Ti ions incorporated in the interstitial sites of hexagonal ZnO lattice. Average crystallite size increased from ~16.63 nm to ~19.08 nm upon Ti doping in ZnO film. Conduction mechanism changed from overlapping large polaron tunneling (OLPT) for undoped ZnO film to correlated barrier hopping (CBH) for TZO film. The experimental data was fitted theoretically using OLPT and CBH models to calculate frequency and temperature dependent DOS. An enhancement of ac conductivity and DOS were observed with the doping of Ti in ZnO thin film. Complex modulus study of TZO film revealed transition from long range mobility to short-range mobility with increase in frequency.

Innovative Computational Approaches for Designing Advanced Optoelectronics Materials towards Energy Applications

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Abstract:

Nonlinear optical (NLO) materials are among the smartest materials of the present era and are employed to modulate the phase and frequency of the laser. The attention of numerous researchers, who are dedicated to discovering new NLO materials suitable for several applications such as second harmonic generation, holographic imaging, telecommunications, laser frequency conversion, quantum computing, quantum optics, plasma physics, and many more. The present study presents a quantum chemical framework for tailoring nitrogen/boron-doped (N/B) derivatives of phenalene and pyrene through terminal and central core modifications to check their NLO properties. The derivatives of these compounds have been designed by introducing various π-conjugated connectors as well as N/B heteroatoms in the phenalene and pyrene rings. Density functional theory (DFT) methods are used to optimize the ground state molecular geometries of designed compounds, represented as Phe-1 to Phe-4 (phenalene derivatives) and Pyr-1 to Pyr-4 (pyrene derivatives) at the M06-2X/6-311G* level of theory. A systematic impact of structural modulations is established by comparing first linear polarizability (α) and second hyperpolarizability (γ). For linear polarizability, Phe-4 has shown the highest value for αiso and αaniso values, which is 114.7 × 10-24 esu and 197.9 × 10-24 esu, respectively. For second hyperpolarizability (γ), among the designed compounds, Pyr-4 has achieved the highest γ amplitude of 1929.9 × 10-36 esu owing to its unique molecular structural design and presence of strong donor-acceptor groups. The origin of higher γ amplitudes is attributed to its lower energy electronic transition, higher oscillator strength. Further analysis of electronic parameters, such as electron density difference (EDD) maps, the density of states (DOS), electrostatic potentials, transition density matrix (TDM) analysis, and frontier molecular orbitals (FMOs) analysis, demonstrated the more effective intramolecular charge transfer (ICT), resulting in a good NLO response. The compounds were also analyzed for their potential in photovoltaic applications based on factors such as open circuit voltage values determined to be

between 2.144 eV to 0.395 eV, and light harvesting efficiency ranging from 0.486 eV to 0.989 eV. These findings suggest that the designed compounds can serve not only as good NLO materials but also possess significant potential for photovoltaic applications.

Comparative Optimization of 3C-SiC and CdS Electron Transport Layers for Enhanced Performance in Sb2S3-Based Solar Cells: A SCAPS-ID Simulation Approach

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Abstract:

In this study, we design a non-toxic, CdS-free thin-film solar cell structure utilizing antimony sulfide (Sb_2S_3) as the absorber material. Sb_2S_3 has proven to be a promising candidate for renewable energy generation. Solar cells based on Sb_2S_3 have attracted worldwide attention due to their outstanding efficiency and low cost. Toxic cadmium sulfide has been replaced with 3C-SiC (cubic silicon carbide) as a buffer layer. 3C-SiC has a larger bandgap compared to CdS, making it more suitable for high-efficiency applications in high- temperature environments. SCAPS-1D (one-dimensional solar cell capacitance simulator) software has been employed to numerically investigate the performance of Sb_2S_3-based n-ZnO/n-3C-SiC/p-Sb_2S_3 heterostructure solar cells. The influence of absorber/buffer layer thickness, acceptor/ donor densities, and defect density on device performance has been investigated. Additionally, the role of defects in p-Sb_2S_3 and the significance of n-3C-SiC/p-$Sb2S_3$ interface defects have been investigated to provide recommendations for achieving high efficiency. The proposed solar cell structure n-ZnO/n-3C-SiC/p- Sb_2S_3 demonstrates an impressive efficiency of 17% under 1.5 G illumination spectrum. The parameters regarding solar cell performance such as Voc, Jsc, FF, QE and η have been studied graphically. This novel structure may have considerable influence on the progress of improved photovoltaic devices in the future.

Poster Session

Efficient Removal of Different Pesticides from Aqueous Media Through Activated Charcoal/ Chitosan Composite

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Abstract:

Growth in population and the resulting greater need for agricultural products have contributed to an uncontrollable increase in the usage of pesticides. Natural ecosystems have shown pesticides to be persistent, causing detrimental effects on human health, plants, animals, and the aquatic environment. Adsorption is an effective method for the treatment of pesticides present in wastewater. Activated charcoal is inexpensive, easily available, and shows high adsorption activity. It is modified with chitosan, which is biocompatible, homophilic, adhesive, non-toxic, exhibiting antibacterial capabilities, cheap, readily available, and possessing adhesive qualities used for the removal of cypermethrin from aquatic media. The surface characteristics, i.e., morphology, physiochemical properties, and structure of the adsorbent, were characterized by using various techniques such as Fourier transform infrared (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM), and point-of-zero charge reactions. Taguchi statistical design of experiment is used for optimizing reaction parameters such as temperature, time, pH, adsorbent dose, and initial concentration. Batch adsorption studies revealed that both pesticides showed a maximum removal efficiency for cypermethrin is 90% and at pH 4. Equilibrium was achieved after 40 min of contact time with an initial concentration of 40 mg/L, temperatures of 40°C, and adsorbent doses of 0.0125 L/mg, respectively. Intraparticle diffusion, pseudo- first-order, pseudo-second-order, Elovich kinetics, Langmuir, and Freundlich isotherms models were used to study the adsorption process. In kinetic and equilibrium studies, pseudo second order and Langmuir isotherm models were best fitted in the adsorption process. Thermodynamics studies showed that the reactions were spontaneous.

Computational Analysis of Ribofuranose Nucleoside Derivatives: Targeting EGFR and VEGFR2 in Cancer Cells

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Abstract:

Anti-metabolites are among the most effective chemotherapeutic agents for cancer treatment due to their ability to disrupt DNA synthesis. Recently, there has been growing interest in modified nucleoside analogues, which have demonstrated superior effectiveness. These nucleoside analogue derivatives are promising candidates for cancer therapy because they specifically target cancer cells. Their selective action on molecular pathways has reduced toxicity and enhanced effectiveness compared to traditional chemotherapy drugs. Nucleoside analogues interfere with the natural function of nucleosides, leading to cytotoxic effects in cancer cells. In this study, derivatives of ribofuranose nucleoside analogues were designed. Density functional theory (DFT) calculations were conducted at the B3LYP/6–311 G(d,p) level, and the molecules were characterized using UV/Vis spectroscopy with the CPCM model in DMSO solvent. Molecular structural parameters, including HOMO/LUMO and MEPS, were also determined. Among the derivatives, d1m demonstrated high energy gap and low absorption energy. Molecular docking studies of the derivatives (d1o-d2m) were performed with the EGFR and VEGFR2 proteins, revealing that d2o had strong binding affinity with EGFR, while d1o showed favourable interactions with VEGFR2. Additionally, global chemical parameters and natural bond orbital (NBO) analysis were employed to examine charge transfer properties and chemical reactivity. NBO analysis identified donor and acceptor regions within the molecules, and global chemical parameters provided insights into their reactivity, stability, and solubility. The results showed that the derivatives are more chemically reactive, thermodynamically stable, and possess better binding affinity than the parent compound. These findings suggest that the interaction of the derivatives with cancer-related proteins enhances their potential effectiveness as cancer treatments.

Nano-suspension Formation of *Amaranthus Viridis* and *Calotropis Procera* to Enhance their Bioavailability

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Abstract:

Nanosuspensions were formed by using herbal drugs, to enhance dissolution rate and bioavailability of Amaranthus Viridis and Calotropis Procera. Precipitation technique was used to prepare nanosuspensions by using SDS (Sodium Dodecyl Sulphate) as a stabilizer. Drugs powder was dissolved in an organic solvent and mixed with stabilizer solution. The mixture will be homogenized to form nanosuspension by using Sonicator. Particle Size Distribution, X-Ray Diffraction (XRD), Saturation Solubility, Dissolution Rate, Stability Test, pH effect, Scanning Electron Microscopy (SEM), Differential Scanning Calorimetry (DSC), Drug Release Profile Study and Fourier Transform Infrared Spectroscopy (FTIR) characterizations were performed for nanosuspensions. The particle size of Amaranthus Viridis and Calotropis Procera was found 230nm and 183nm, respectively. The nanosuspensions showed improved dissolution and stability under cold conditions. This study illustrated that developed nanosuspension had great approach to improve herbal drugs solubility and enhanced bioavailability.

Removal of Pesticides from Aqueous Solution with Magnetic Chitosan Grafted Salicylaldehyde/ Nano Clay Composite

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Abstract:

Several pesticides are utilized to control pests in agricultural fields for better and maximum yield of agricultural products due to their increasing demand. These pesticides have adverse effects after releasing into environmental components like soil, water and air. Adsorption is an attractive approach for the treatment of wastewater containing pesticides. In this work, magnetic chitosan Nanoclay grafted Salicylaldehyde adsorbent was prepared for the removal of paraquat pesticide. The adsorbent was prepared with magneto-responsive behavior and easy separation due to the presence of iron oxide nanoparticles. When chitosan, Salicylaldehyde, iron oxide and Nano clay work together their working efficiency and mechanical stability significantly increase. This composite was characterized by Fourier transfer infrared spectroscopy (FTIR), scanning electron microscopy-energy dispersive X-ray (SEM-EDX), powder X-ray diffraction (XRD) and point of zero charge reaction. Taguchi statistical design was used to optimize several adsorption affecting parameters. The optimized conditions are the adsorbent material 0.01g/mL, pH 7, contact time 40 mints, concentration of pesticide solution of 100mg/L and temperature with a 96% removal efficiency and 483 mg/g adsorption capacity. To understand the adsorption mechanisms kinetic, equilibrium, and thermodynamics studies were conducted under the optimized conditions. The adsorption mechanism was kinetically fitted to a pseudo-second-order model and isothermally fitted to a Langmuir model. The negative value of ΔG° and positive values of ΔH°, Ea, and ΔS° indicated the spontaneous, endothermic nature of the adsorption process with an increase in randomness as adsorption precedes respectively. Optimizing the adsorption parameter by the Taguchi design proved effective for removing Paraquat pesticides using prepared adsorbent.

Eco-Inspired Nanoparticles: Rice Husk-Derived Zinc Oxide for Promoting Coriander Growth

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Abstract:

Nanotechnology emerges as significant research discipline in the scenario of modern research with potential applications in numerous fields. Green nano-engineering spotlight on developing procedures which are clean, safe and particularly environment friendly in contrast to chemical and physical methods for nano-synthesis. Nanotechnology has potentially effective impact regarding precision agriculture. Many advance research fields like plant protection, nutrition and farm particles management make use of nano-agrochemicals. Engineering ZnO nanoparticles is the domain of interest for research due to their remarkable features like size, electrical, magnetic and optical properties. Present study focus on the green synthesis of ZnO nanoparticles using rice husk. Characterization of zinc oxide nanoparticles done by using UV Visible spectroscopy, FTIR, SEM and XRD. The study was investigate the fast and ecofriendly application of synthesized nanoparticles in the field of agriculture. The data obtained was be subjected to statistical analysis by using appropriate statistical tools.

The Photocatalytic Degradation of Textile Dyes using Green Synthesized Zinc oxide Nanoparticles

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Abstract:

The wastewater produced during dyeing process in textile industries contains various chemicals and toxic dyes which are causing significant threats to our environment. Industries are releasing untreated dyes into water bodies, therefore; wastewater needs to be treated properly before its disposal. Photocatalysis is one of the best practices for degradation of dyes in wastewater. The photocatalytic nanoparticles synthesized using green method has become a great deal of attraction due to their cost effectiveness, ecofriendly behavior and high efficiency. They bind dye on their surface, adsorb it and convert into smaller non-toxic substances by irradiation of sunlight. The aim of this study was the green synthesis of zinc oxide nanoparticles using natural plant leaf extract as reducing agents. The synthesized nanoparticles were characterized by various techniques such as Zeta-sizer, SEM and UV-Visible spectroscopy. The photocatalytic efficiency of synthesized nanoparticles was evaluated against two synthetic textile dyes; direct blue and direct violet. 90% removal of direct blue 297 was observed at temperature 55°C, pH 7, incubation time (120 mins), nanoparticles concentration 0.02g and dye concentration (60ppm). However, 87% removal of direct violet 66 was observed at temperature 60°C, pH 7, incubation time (120 mins), nanoparticles concentration 0.02g and dye concentration (50ppm). ZnO nanoparticles showed broad temperature and broad pH hence it can be a best candidate for treatment of real textile effluents.

Potential of *Mangifera indica* Biomass based Na-alginate and Hybrid Composites for the Removal of Imidachlopride from Wastewater

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Abstract:

Adsorption is considered the most propitious and dynamic technology for the detoxification of water from noxious pollutants. Present research work was premeditated to use Mangifera indica (mango) seed shell and its composites for the removal of organic pollutants such as pesticides imidacloprid, from wastewater. Composites prepared by Native Biomass were Biomass Magnetic composites (BMc), and sodium alginate Na-alginate composites. After synthesis different analytical techniques, SEM-EDS, XRD, FTIR and TGA-DSC were used for the characterization of composites and biomass before and after adsorption experiments. The batch experimental study illustrates the optimum pH for imidacloprid was in acidic range with BM composites and neutral with Na-alginate. Similarly, RG-5 and D. sodium was well adsorbed in acidic media with all adsorbents. On increasing biosorbent dose adsorption capacities were found to be decreased with both composites. Optimum temperature for adsorption of Imidacloprid were 60 oC (Na-alginate) and 30 oC (BMc), maximum adsorption for Imidacloprid were obtained in 2 hours (120 min) BMc and 1.5 hours (90 min) with Na-alginate composites. Kinetic (pseudo first-order, second-order and intraparticle models, second-order and intraparticle) and Equilibrium Langmuir, Temkin, Freundlich, Harkins-Jura and Doubinin-Radushkevich) models were applied on the batch experimental data. Langmuir, D-R and Temkin showed fitness on experimental data. Models were applied on the batch experimental data. Thermodynamic parameters were also calculated to evaluate the nature and the feasibility of adsorption reaction. This experimental work revealed that the use of biocomposites as compared to native biomass is a suitable option for the exclusion of pesticides from contaminated water.

A Field Portable Electrochemical Immunosensor based on Multifunctional Ag_2O/G-C_3N_4 @MA-DBB Covalent Organic Framework Receptor Interface for Single-Step Detection of Aflatoxin M_1 in Raw Milk Samples

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Abstract:

Aflatoxin M_1 (AFM_1), a Group II-B carcinogen in milk, originates from the ingestion of *Aspergillus*-contaminated feed by livestock. To address the need for an easy-to-handle, sensitive, and portable detection method, we developed an electro-active nanocomposite immunosensor using Ag_2O/g-C_3N_4-COOH@MA-DBB-COF (silver oxide/carboxy-functionalized graphitic carbon nitride@melamine-dibromo butane COF) as a multifunctional receptor. This immunosensor demonstrated a linear AFM_1 detection range of 0.03–1000 fg mL^{-1} and a detection limit of 0.01 fg mL^{-1}, with high selectivity in anti-interference tests. Practical application was validated through AFM_1 detection in real milk samples with recoveries of 97.28–102.62. This study introduces a single-step, field-portable, label-free electrochemical immunoreceptor for on-site AFM_1 detection in milk samples.

Bioremediation of 2, 4 dichlorophenoxyacetic acid from Simulated Wastewater by Magnetically Active and $NABH_4$ based Hybrid Composites

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Abstract:

The project was planned to investigate the potential of commonly available agricultural wastes to remove/adsorb the pesticides such as 2,4 dichlorophenoxy acetic acid (2,4, D)from wastewater. Study of screening trials showed that mango stones shell based biomass have maximum removal potential to adsorb pesticides from simulated wastewater. During batch study, different process parameters like pH, biosorbent dose, contact time, initial dye concentration and temperature were optimized. Effect of surfactants, salts and heavy metal ions was also investigated. The maximum pesticides removal was observed in acidic range of pH with 0.05 g with both Magnetic biomass (MBc) and Na-hybrid composites. The results of batch study showed that, biosorption is a rapid process and equilibrium was attained in less than 90 minutes. The kinetic data fitted well to the pseudo-second-order kinetic model. During the initial dye concentration trial, it was observed that magnetically active and hybrid composites have the potential to adsorb 2,4,D from wastewater. Different models (Langmuir, Freundlich, D-R model, Herkins Jura and Temkin adsorption isotherms) were applied to the equilibrium data. Biosorption seemed to be an exothermic process and increasing temperature reduced the biosorbent adsorption potential of Na-hybrid composites but the MBc showed endothermic adsorption phenomenon and have high adsorption potential even at 50°C . The maximum Pesticides 22.5 mg/g and 29.33 mg/g was observed at 25°C and 50°C respectively with Na-hybrid and MBc composites. Thermodynamic parameters i.e., Gibbs free energy (ΔG°), enthalpy (ΔH°) and entropy (ΔS°) were also calculated.

Salen Based Metal-COF and Cobalt Ferrite Decorated Electrochemical Sensor for the Detection of Atrazine in Ground Water

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Abstract:

Atrazine, a widely used herbicide, poses significant environmental and health risks due to its persistence in water sources, necessitating the development of efficient and sensitive detection methods. This study introduces a novel electrochemical sensor based on a $CoFe_2O_4$/Fe-PaTp-COF hybrid nanocomposite for the selective detection of atrazine. The hybrid material was thoroughly characterized using SEM, FTIR, TGA and XRD, confirming its hierarchical structure and chemical integrity. Electrochemical techniques, including cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS), revealed enhanced conductivity and improved electron transfer kinetics. Differential pulse voltammetry (DPV) in 2M KOH demonstrated an exceptional detection limit of 2.5 ppb, with linear calibration ranges of 0.0139–2 μM and 20–300 μM. The sensor exhibited a recovery rate of 97% in groundwater samples, along with excellent stability and reproducibility. This work offers a sustainable and highly sensitive platform for atrazine detection in ground water, contributing to advancements in environmental monitoring technologies.

Efficacy of Soil and Foliar Applications of Chemically Synthesized Zno Nano Fertilizer on Morphological and Nutritional Quality of *Zea Mays* Crop: A Comparison

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Abstract:

The primary goal of using Nano-fertilizers in agriculture is to reduce mineral fertilizer losses while increasing yields to promote agricultural output. In this context, the present study was conducted at Post agriculture research station (PARS) UAF, in the growing season of maize plant to investigate the efficacy of chemically synthesized Nano fertilizer of Zinc on the biochemical, morphological, physiological, nutritious quality and yield related parameters of maize. Despite the fact that ZnO is commonly researched on plats in many types of soils, the soil contains numerous nutrients, including some of the toxic components that might influence ZnO studies. As a result, the current investigation was conducted in double washed sand to remove all sand nutrients and components. The Zinc nanoparticles were synthesized chemically and characterized to investigate the size, surface morphology, dimensional structure and crystalline composition using SEM, XRD, FT-IR, and UV-Visible spectroscopy. The Nano-fertilizers were applied to plants using two techniques, through soil application and foliar application. For soil application, a maximum average increase of 61.1% in plant growth, 51.8% in photosynthetic pigments and 49.25% in anti-oxidant contents was observed as compared to control plant. For foliar application, an average increase of 59.28% in plant growth, 48.19% in photosynthetic pigments and 52.91% in anti-oxidant contents was observed as compared to control. The results suggests that, the ZnONPs have the potential to be employed as a Nano fertilizer for crops cultivated in Zn-deficient soils to boost agricultural output, food quality, and alleviate worldwide hunger.

Evaluation of Nutritional, Bioactive, wound healing and antitumor potential of *Ficus Carica*

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Abstract:

The common fig tree, Ficus carica, is a native of southwest Asia and the eastern Mediterranean and was one of the earliest plants that people cultivated. The harvest of figs is crucial for both their fresh and dry consumption globally. Ficus carica have long been valued, Because of its capability to treat a number of illnesses. This study assesses the phytochemicals, antioxidant activity, wound healing, antibacterial activity anticancer, and cytotoxicity of two types of dried fig and one type of leaf extracts of Ficus carica. Techniques like Folin-Ciocalteu, Aluminium Trichloride, and Bradford were used to determine the extracts total phenolic, flavonoid, and protein contents. High-performance liquid chromatography (HPLC) was used to characterize the extracts further. Traditional medicine has used Ficus carica for various diseases, and further investigation is crucial to explore its potential as a medicinal agent.

A Safe Trash to Treasure Approach: Upcycling PPE Waste into Lead-Removing Multifunctional Material through Pyrolysis

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Abstract:

Lead contamination in water poses severe health risks, necessitating urgent and effective remediation strategies [1]. This study explores the use of carbon-based materials derived from the co-pyrolysis [2] of PPE waste and agricultural residues [3] as efficient adsorbents for lead ion removal. The surge in PPE [4] usage during the COVID-19 pandemic has exacerbated plastic pollution, highlighting the need for innovative waste management solutions. Co-pyrolysis transforms PPE and biomass into biochar with enhanced adsorption properties, offering a dual benefit of waste mitigation and resource generation [5]. Our findings demonstrate that pyrolyzed carbon achieves up to >95% lead removal from 50 ppm solutions within 50 minutes, showcasing its rapid and efficient performance. This approach aligns with global sustainability goals by simultaneously addressing plastic pollution and improving water quality. By converting PPE waste into high-performance adsorbents, this research highlights the potential of co-pyrolysis in advancing sustainable wastewater treatment technologies. Optimizing this process could further enhance lead removal efficiency, paving the way for innovative solutions in environmental remediation and sustainable waste utilization.

Synthesis of Biomolecules-Capped Silver and Iron Oxide Nanoparticles for Advanced Antimicrobial Therapies

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Abstract:

Pseudomonas aeruginosa and Staphylococcus aureus are hazardous biofilm-forming bacteria, posing significant challenges due to their antibiotic resistance [1]. In this study, Rhamnolipid (RL)-coated silver (Ag, 35 nm) and iron oxide (Fe_3O_4, 48 nm) nanoparticles (NPs) were synthesized using a facile method and evaluated for their antibacterial and anti-biofilm properties. These RL-coated NPs effectively inhibited biofilm formation and disrupted pre-formed biofilms of both strains. Mechanistically, the NPs generated reactive oxygen species [2] and reduced cell adhesion by altering surface hydrophobicity, enhancing their anti-biofilm activity. These findings highlight the potential of RL-coated Ag and Fe_3O_4 NPs for biomedical applications, such as antibacterial coatings and wound dressings.