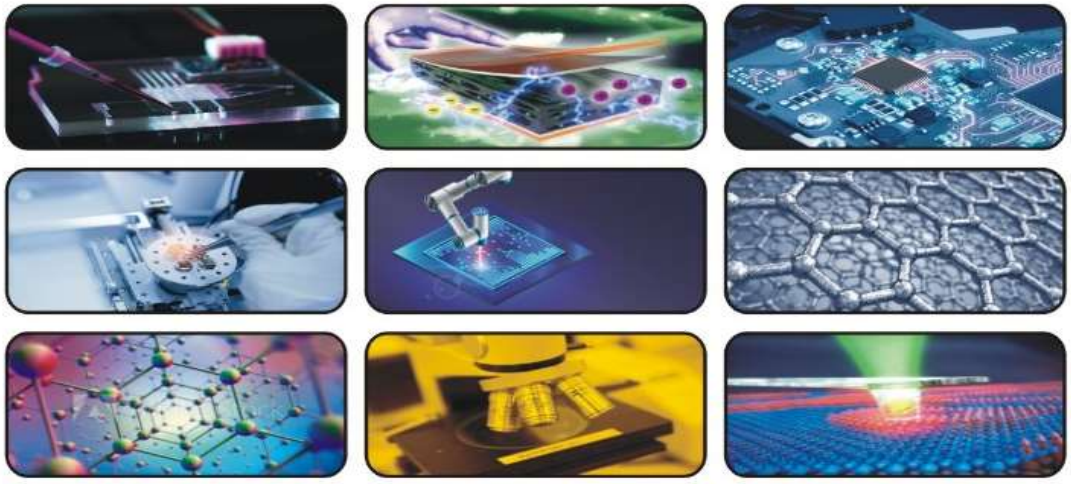
6th International Conference On Materials Science & Nanotechnology 2023



Abstract Book

MSNANO23

September 25-27, 2023

Organized By:

Nano-Materials and Biosensing Research Center (NBRC)

Department Of Physics

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Sponsored By:

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Message from Vice Chancellor

It is a matter of great pleasure that **Nanomaterials and BioSensing Research Center (NBRC) Department of Physics** is organizing an International Conference on Materials Science and Nanotechnology & International Hand On Training/Workshops annually since 2017. This conference is a step towards achieving our vision in becoming a world class academic and research institution. In last couple of years, Government College University, Faisalabad is endeavoring to uplift its research environment and establishing international linkages and collaborations. This event is a great opportunity for the researchers of GCUF as well for researchers from other universities of Pakistan to share their ideas and interchange knowledge with the top class scientists from advanced countries in the fields of materials science and nanotechnology. I am very certain that this event will be able to provide a platform towards strengthening out collaborations and bosting research activities in GCUF.

At the end, I would like to congratulate the Department of Physics for their commitment and superb drive to organize this mega event. It is my aspiration that this conference will be a foundation for the growth of new ideas towards a better tomorrow.

Message from Dean

I feel pleasure to welcome all the international and national guests on the occasion of 6th International Conference on Materials science and Nanotechnology (MSNANO-2023). I am confident that MSNANO-2023 just like previous three events will play important role in boosting research activities at GCUF and research collaborations with international partners especially from technologically advanced countries. It is pertinent to mention here that Department of Physics has shown tremendous progress in recent couple of years in research and academia. Research laboratories established in department of Physics are of International standards and producing highly skilled researcher scholars. MSnano-20 is a platform that provides opportunity to our students and researchers to get new ideas and to make their research more fruitful for the country.

I would like to express my sincere gratitude to the distinguished invited speakers for their presence and contributions to the conference. I also thank all the program committee members for their efforts in ensuring a rigorous review process to select high quality papers.

Finally, I sincerely hope that all the participants will benefit from the technical contents of this conference, and wish you a very successful conference and an enjoyable stay in Faisalabad.

Message from Chairman Department of Physics

Department of Physics, Government College University, Faisalabad has emerged as a leading center of learning and research in a short span of time. Department of Physics with its dynamic faculty and innovative syllabi has become a catalyst of intellectual, social and industrial change.

The Department of Physics is imparting quality education and research guidance to its students with the aim of serving the community at large. We have more than 30 faculty members striving arduously for achieving excellence in their profession and are utilizing all their potential to the maximum for uplifting the academic and research standards of the University.

The diversity of the existing research expertise in the Department of Physics would provide prospective students with deep and interdisciplinary knowledge; and would enable them to acquire technical skills that make them uniquely competitive.

Department of Physics has rich history of organizing International conferences, workshops and symposiums every year and ***6th INTERNATIONAL CONFERENCE ON MATERIALS SCIENCE & NANOTECHNOLOGY (MSNANO-2023)*** is one of these prestigious events.

The main objective of ***MSNANO-2023*** conference which is going to be an elite event is to network with your peers from academia and industry:

Key Features of *MSNANO-2023* are:

- The Scope *of MSNANO-2023* includes Materials Science/ Nanotechnology/ Polymer Science/Biotechnology/energy devices and modeling and simulation.

- Interaction with World Renowned Speakers & Panel Discussions,
- Interactive Poster Session,
- Emerging Researcher Forum,
- Networking & Collaboration,
- Target Audience: Research Professors/Students/Physicists/Chemists/research fellows and industry.

I am hopeful that ***MSNANO-2022*** will prepare students to think rigorously and conduct meaningful and cutting-edge research, preparing them for fulfilling careers in academia

I would like to invite participants across the globe to attend the *MSNANO-2023*, which is to be held in **25-27 September, 2023** at Quaid-e-Azam auditorium Government College University Faisalabad, Pakistan, for prompt Keynote Presentations, Oral Talks, Poster Competition and Exhibitions.

I also invite you to spare some time to visit our department to learn more about the latest research, achievements, expertise and events. Even better, I encourage you to visit our laboratories in person, to meet our students and faculty and be inspired by the innovation, ambition, and creativity you will find here.

Preface

Government College University Faisalabad since 2002 has provided a platform for the research atmosphere though various approaches. One of them is to organize International & National Conference, Seminars to bring the scientists from Research & Development organization, Research Institutes, Universities to interact and work on the problems of applied nature to provide solutions. In the same spirit, department of Physics has started the International Conference on Materials Science & Nanotechnology since 2017. The purpose of this conference is strengthen the research atmosphere at the department of Physics where faculty and students can address the problems of Industry and provide simple and cheap solutions to these. In the 1st MSNAON-17, Professor Dr Ya-Hong Xie, Dr Jimmy and many eminent speakers presented their work. That conference resulted in a joint Pak-US research project of Dr. Khalid Mahmood and Prof Dr Ya-Hong Xie on the development of biosensing chips for the detection of bacteria in in blood for the rurual areas of Pakistan. In 2nd MSNANO-18, Professors from University of Saint Andrews, University of California Los Angeles, University of Peking China come to GC University Faisalabad and presented their work. 3rd MSNANO-19 attracted the attention of many eminent researchers of Pakistan where speakers from 40 different universities come to present their work besides the speakers from USA, UK, China, Turkey, Saudia Arabia and Korea. In 4th MSNANO-20, speakers from University of Waterloo, University of Saint Andrews, South bank London University, University of North Carolina Charlotte, University of California Los Angeles are participating and more than 200 abstracts are received. Conference proceedings shall be published in; Physica B: Condensed matter Physics (IF; 1.8), Journal of Superconductivity and Novel Magnetism (1.1), Materials Today: Proceedings and Springer Conference series on Materials shall be publish the oral and poster presentations.

ABSTRACT BOOK

6th INTERNATIONAL CONFERENCE ON

MATERIALS SCIENCE & NANOTECHNOLOGY (2023)

MSNANO-23

About/Introduction

Advances in synthesizing smarter and efficient nano-materials for various technological applications are directly related to the development in nano-technology. The proposed international event aims at bringing together renowned scientists of international eminence and to exchange their knowledge and ideas in cutting edge Nano-materials technology for future applications including Nano-electronics, Nano-mechanics, Nano-medicine and especially Nano-energy.

Mission

The aim and objective of MSNANO-2023 is to provide a platform for researchers, engineers, academicians as well as industrial professionals from USA, China, Singapore, Saudi Arabia, United Kingdom, South Korea, Pakistan and Turkey to present their research results and development activities in the functional applications of nano-materials for energy and electronic applications. This conference provides opportunities for the delegates to exchange new ideas and applied experiences, to establish research as well as commercial relations and to find global partners for future collaboration. The research students working on state of the art nano-technologies will get a chance to share their problems with renowned scientists of technologically advanced countries. Moreover, the platform may also help in uplifting the interest of local investors for advancing local manufacturing of nano-materials for various applications.

Conference Topics

Semiconductor Materials	Materials for energy Storage
Photovoltaic	Fuel Cells Materials
Organic Solar Cells	Nuclear Energy
Silicon Solar Cells	Thin Films for Energy
Thermooelectrics	Catalysis, Photocatalysis
Nanostructures	Smart Materials for Energy
Semiconductors	Nano-materials for energy
Nano-ferrites	Graphene
Nano-Materials	2D Materials
Optoelectronic Devices	Other related topics
Nanomedicine in pharmaceutics	

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Program

6th International Conference on Materials Science and Nanotechnology 2023

(MSNANO-23)

	Day 1 **25 September, 2023**		
08:00-09:30	Registration		
09:30-10:40	**Inaugural Session**		
09:30	Guests to be seated		
09:30-09:40	Recitation from the Holy Quran & Naat-e- Rasool (P.B.U.H)		
09:40-09:50	**Remarks: Special Guest; Ms. Warda Dar, British Council, Pakistan**		
09:50-10:30	**Plenary talk: Prof. Dr. John Buckeridge (London South Bank University, UK)** *Insights into fundamental processes in energy materials from computational modeling*		
10:30-10:40	**Remarks: Chief Guest; Prof. Dr. Nasir Amin, Principal Organizer and Vice Chancellor, Government College University Faisalabad**		
10:40-11:10	**Refreshment Break**		
	Parallel Session I **Quaid-e-Azam Auditorium, Hall I**	**Parallel Session II** **Quaid-e-Azam Auditorium, Hall II**	**Parallel Session III** **STC Hall III**
	Session Chair: **Dr. M-A Hassan (UNCC, USA)**	**Session Chair:** **Dr. M. Isa Khan (IUB, RY Khan)**	**Session Chair:** **Dr. M. Asghar Hashmi (NSU,**

			Islamabad)
11:10-11:40	**M. Aslam Baig (H.I, S.I, T.I) (QAU, Islamabad)** *A Comparative Study of Materials Analyses using LIBS and Other Analytical Techniques*	**Altaf Hussain (IUB, Bahawalpur)** *Ab-Initio Investigation of Novel Multi-functional Half-Heusler Compounds*	**Zafar Hussain Ibupoto (UoS, Jamshoro)** *Nanostructured Materials for Green Energy, Environment, and Electroanalytical Applications*
11:40-12:00	**Tariq Sajjad (LSBU, UK)** *Light Harvesting in Organic Solar Cells*	**Nasir Rasool (IUB, Bahawalnagar)** *A Comparative Study of Different Physical Properties of Nowotny Phase TM5Si3C (TM = Nb, Mo) Ternary Silicides*	**Sadia Muniza Faraz (NED, Karachi)** *Low-Cost Manganese Oxide Counter Electrode for DyeSensitized Solar Cells by Repurposing Wasted Battery Cells*
12:00-12:20	**Zunaib Ali (LSBU, UK)** *Modeling and Control of Grid-connected Renewable Energy and Electric Vehicular Systems for Smart Grid Applications*	**Amir Rafique (IUB, Bahawalpur)** *First-principles study on the structural, mechanical, electronic structure, thermal and thermophysical properties of XS (X = Ge, Sn, Pb) monochalcogenides*	**Anila Tabassum (PU, Lahore)** *Cu/Co bimetallic oxides for understanding oxygen evolution reaction (OER) of electrochemical water splitting*
12:20-12:40	**Waqas Zulfawar (Namur, Balgium)** *Structure inversion asymmetry enhanced electronic structure and electrical transport properties in anti-perovskite monolayers: A first-principles study*	**M. Irfan (GCUF, Faisalabad)** *Hydrothermal synthesis and characterization of CoCrAl Heusler alloys*	**M. Azhar Khan (IUB, Bahawalpur)** Investigations of physico-chemical, structural and dielectric features of Gd3+ substituted Ba2Zn2Y Hexa-Ferrites for high frequency absorption applications
12:40-13:00	**Sadia Z Bajwa (NIBGE, Faisalabad)** *Advanced Nanotechnology-based Biosensors; Characteristics and*	**Dilbar Iqbal (PINUM, Faisalabad)** *Development of Novel Deep Learning-Based Segmentation Models using MRI images for Low-Grade Glioma Brain Tumor*	**Bin Amin (AUST, Abbotabad)** *Two-Dimensional Transition Metal Dichalcogenides with*

	Prospects	*segmentation*	*Tailored Properties*
13:00-13:15	**Pervaiz Ahmed (AJKU, Muzafarabad)** *Hexagonal Boron Nitride nanomaterials; synthesis, characterization and potential appliations*	**Faiq Sabir (GCUF, Faisalabad)** *Green synthesis of ago nanoparticles with azadirachta indica and turmeric roots for antimicrobial applications*	**Sami ur Rehman (Riphah University, Faisalabad)** *Synthesis, Preparation and Properties of 2D-Graphene for Electrochemical Energy Storage and Conversion*
13:15-14:30	**Lunch**		
	Session Chair: **Dr. Abdul Khaliq Jan (SBBU, Dir)**	**Session Chair:** **Dr. Sajad Hussain Bhatti (UE, Joharabad)**	**Session Chair:** **Dr. M. Bilal Tahir (KFUEIT, RY Khan)**
14:30-15:00	**Muhammad Faryad (LUMS, Lahore)** *Introduction to Quantum Computing*	**Ejaz Muhmad (AIOU, Islamabad)** *Bi_2O_3/WO_3 Heterostructure as Efficient Solar Driven Photocatalyst*	**Javaid A Bhatti (IVC, Islamabad)** *Improvement in the pumping technique of the molecular drag pump*
15:00-15-20	**Ghulam Asghar (University of Ponch, Rawalkot)** *Structural, morphological and magnetic properties of M-type hexaferrites*	**M. Irsam (Italy)** *Unveiling the Thermoelectric Performances of Zn1-xFexSe Nanoparticles Prepared by the Hydrothermal Method*	**Amir Ullah (ICU, Peshawar)** *High strain response and ferroelectric properties of Bi1/2Na1/2TiO3 based perovskites*
15:20-15:40	**K.M Zia (GCUF, Faisalabad)** *Future of Polymer Industry: A Spectrum from Bionanocomposites to Energy Harvesting Applications*	**Sabira Sultana (GCUF, Faisalabad)** *Green Metal Nanoparticles: An Eco-Friendly Approach for Advancing Cancer Treatment*	**Malika Rani (Women University, Multan)** *Enhanced Supercapacitor Performance through Synergistic Synthesis and Electrochemical Characterization of NdCrO3/GO Nanocomposite*
15:40-16:00	**Zahir Iqbal (GIKI, Topi)** *Supercapacitors and batteries: A critique of popular cyclic*	**Rabia Naeem (GCUF, Faisalabad)** *Binary and ternary mixed metal oxide thin films fabrication by AACVD for*	**Azka Kanwal (GCUF, Faisalabad)** *Synthesis and electrochromic evolution of graphene quantum dots/polyvinyl alcohol*

	voltammetry diagnostic model to deconvolute capacitive and diffusive contributions	*optical and Solar water splitting*	
16:00-16:20	**Waheed S Khan (NIBGE, Faisalabad)** *Large Scale Production of Nanomaterials from Cheaper Sources for Useful applications in Agriculture and Environment*	**Misbah Shaheen (GIKI-Topi)** *Metal-organic frameworks for supercapacitor-battery hybrids*	**Shahbaz Rana Muhammad (China)** *Influence of distances between lens to Al sample surface on laser-induced breakdown spectroscopy*
16:20-16:40	**Dr. Ghulam Nabi Watto (UoG, Gujrat)** *Two Dimensional (2D) Hexagonal Nano-sheets as Potential Nano-structures for Energy Storage Devices"*	**Asma Khizar (GIKI, Topi)** *Redox active pyridine-3,5-di-carboxylate- and 1,2,3,4-cyclopentane tetra-carboxylate-based cobalt metal–organic frameworks for hybrid supercapacitors*	**Arooj Anwar (GCUF, Faisalabad)** *Synthesis of silver nanoparticles using green matrix and its application in medical field*
16:40-17:00	**Abdul Hameed Khan (AJKU, Muzafarabad)** *Biomedical and photocatalytic dye degradation studies of Cymbopogon citratus mediated copper oxide nanoparticles (CuO NPs)*	**M. Sohail Akbar (IUB, Bahawalpur)** *Theoretical investigations of the structural, elastic, electronic, magnetic and thermoelectric properties of MRh2O4 (M = Mg, Mn, Cd) spinels.*	**Vaneeza Javed (GCUF, Faisalabad)** *Development Of Technecium-99m Labeled Nanoparticles Loaded With Antimicrobial Agent As Spect Imaging Agent*
17:00-17:15	**M. Irfan (IUB, Bahawalpur)** *Magnetic properties of Ni/BiFeO3 hybrid nanostructures*	**M. Waseem Imtiaz (UAF, Faisalabad)** *Silver supported TiO2 Based Nanocomposite for Efficient Round-the-clock Photodegradation of Methylene blue Wasted Water*	**Adnan Ahmed (PU, Lahore)** *Effect of Fe co-doping on the structural and optical properties of Co:ZnO nanoparticles*
17:15-	**M. Naveed Anjum**	**Shahzaib Khan (GCUF,**	**Busra Sana Idrees (GCWU,**

17:30	**(GCUF, Faisalabad)** *Photocatalytic degradation of Direct Red 28 by Polyorthoanisidine/g-C3N4/TiO2 ternary composite*	**Faisalabad)** *Facile synthesis of CuAl2O4/rGO nanocomposite via the hydrothermal method for supercapacitor applications*	**Faisalabad)** *Diagnostic of breast cancer based on serum and blood analysis using machine learning tools on spectroscopic data*
17:30-18:00	**Tea**		

Day 2
26 September, 2023

	Parallel Session I **, Hall I**	**Parallel Session II** **Quaid-e-Azam Auditorium, Hall II**	**Parallel Session III** **STC Hall III**
	Session Chair: **Prof. Dr. Syed Zafar Ilyas (AIOU, Islamabad)**	**Session Chair:** **Dr. G.N Wattoo (UoG, Gujrat)**	**Session Chair:** **Dr. Shafaqat Hussain (UoB, Sakardu)**
09:30-10:00	**M. Hassan Sayyad (GIKI, Topi)** *Laser Ablation: Fundamentals and Applica tions in Research & Materials Processing*	**Nadeem Abbas (UAF, Faisalabad)** *Synthesis and Characterization of Ga2O3 Thin Films Deposited on Si(110)*	**Hammadullah (BUITS, Quetta)** *Plasma Technology as a Sustainable source for Environmental Protection*
10:00-10:15	**Abdul Ghafar Wattoo (KFUEIT , RY Khan)** *One-step Fabrication of Nanophotonic Structures: Wide band Absorbers*	**Nosheen Kanwal (GCUF, Faisalabad)** *Optical and dielectric study of synthesized PVDF-based TiO_2 /ZnO nanocomposites*	**Akhlaq Ahmed (UoP, Peshawar)** *Synthesis and characterization of tin (sn) doped nizn*

			ferrite nanoparticles for its application in gas sensor
10:15-10:30	**M. Tariq Qamar (FCCU, Lahore** *Photocatalysis- from designing of Nanostructures to Environmental and Energy Applications*	**Ama Tul Zahra (GCUF, Faisalabad)** *Strained Mechanical Analysis of Carbon Nanotube Using Molecular Dynamics Simulations*	**M. Danish Khan (UET, Lahore)** *Enhancing Methylene Blue Photo-degradation with Silver-Doped ZnO Nanoparticles*
10:30-10:45	**Zahir Gilani (BUITMS, Quetta)** *Application of nano-magnetic particle: Industrial, medical and environmental use*	**Sobia Zareen (GCUF, Faisalabad)** *Radio sensitization Effects of Gold Nanoparticles in Proton Treatment*	**Iqra Fareed (UET, Lahore)** *Insight into Methylene Blue removal using ZnO/Co_3O_4 Photocatalyst*
10:45-11:10	**Tea**		
	Session Chair: **Prof. Dr. Hassan Sayyad (GIKI, Topi)**	**Session Chair:** **Prof. Dr. Ayaz Arif (AJKU, Muzafarabad)**	**Session Chair:** **Prof. Dr. Zafar Hussain Ibupoto (UoS, Jamshoro)**
11:10-11:25	**Dilawar Ali (GCU, Lahore)** *Spray Pyrolysis: Crafting Multifunctional Coatings for Wettability, Photocatalysis, Antimicrobial Efficiency, and Supercapacitor Electrodes*	**Kinza Zulfiqar (UAF, Faisalabad)** *Investigation of Cr_3 Doped $CuGao_2$ as an inorganic Hole Transport Material (HTM) for Perovskite Cells*	**S. Manzoor (NTU, Faisalabad)** *Experimental and Theoretical Study into the Morphological, Vibrational and Optical Characters of Al_2O_3, CuO and ZnO-based nanofluid*

11:25-11:40	**M. Inshad Khan (IICS, Rawalpindi)** *Synthesis and Characterization of Oligoimide-Grafted Graphene Oxide-Epoxy Nanocomposites with Improved Thermal and Mechanical Properties*	**Adil Shahbaz (UAF, Faisalabad)** *Laser-induced breakdown spectroscopy coupled with machine learning for identification of ionization states of oxide materials*	**Ghulam Murtaza (IUB, Bahawalpur)** *Structural, Electronic, Optical, Mechanical, Thermodynamic and Thermoelectric Properties of $ZnSnN_2$ and $ZnMoN_2$ Ternary Nitrides*
11:40-11:55	**M. Afzal Khan (IUB, Bahawalpur)** *Leading role of Nanotechnology for Finding the Effective Ways of Diagnosis and Treatment of Diseases*	**Maria Khalil (PU, Lahore)** *Epsilon-near-zero Response in Magnetron Sputtered Al-substituted Titanium Oxynitride Thin Films*	**Noor ul Ain (IUB, Bahawalpur)** *Photocatalysis of CuO thin film Via Water splitting for Hydrogen generation*
11:55-12:10	**Iqra Muneer (UET, Lahore)** *Advancing Photocatalysis through Hydrothermally Synthesized Metal Oxide Nanoparticles*	**Toba Zareen (UAF, Faisalabad)** *Effect of external fields on synthesis of laser ablated gold nanoparticles and study of their photothermal response*	**Ayesha Javaid (PU, Lahore)** *Bismuth doped cerium ferrite: An efficient material as photocatalyst and dielectric material*
12:10-12:25	**Ghulam M. Mustafa (UE, Faisalabad)** *Temperature Dependent Studies of Ho-Doped Cu-Co Spinel Ferrites Based Graphene Composites*	**Aqeel ur Rehman (UAF, Faisalabad)** *Polar wood modification by ethylene Glycol dispersion*	**M. Faran Yunus (UET, Lahore)** *Bandgap Tunning of Zinc Oxide Heterostructure for Improved Photocatalytic Performance under Solar Irradiation*
12:25-12:40	**Samiullah (BUITMS, Quetta)** *Optical and magnetic studies of $Co_{0.7}Zn_{0.3}Fe_2O_2$ spinel ferrites With*	**Tasmea Nouren Kousar (UAF, Faisalabad)**	**Syed Anwar Hussain Shah (UAF,**

	Dy3+substituted for the application of sensors prepared through sol-gel process	*Synthesis and Characterization of Zr/CeO_2-Based Nanocomposites for Optoelectronic Devices*	**Faisalabad)** *Hydrothermal synthesis, characterization and photocatalytic performance of Carbon quantum dot supported CeO2 photocatalysts*
12:40-12:55	**Hidayat Ullah Khan (UoP, Peshawar)** *Synthesis and Structural Characterization of (LixAg1-x)TaO_3*	**Mumtaz Hussain (GCUF, Faisalabad** *Study of Structural and Optical Properties of Carbon Nanostructures*	**Huda Noor (UAF, Faisalabad)** *Analysis of blood serum using Laser Induced Breakdown Spectroscopy coupled with machine learning*
12:55-13:10	**Asma Hayyat (GCU, Lahore)** *Nanosecond Laser Irradiance-Based Growth of Surface Structures on Si and Ge Correlated With Plasma parameters*	**Abuzar Husnain Raza (UAF, Faisalabad)** *Optical, Structural, and Morphological Properties of Ag-doped CuO Nanoparticles*	**Sajjid Hussain (UAF, Faisalabad)** *Optimizations of Zr/rGO/CeO_2-Based Nanocomposites for Optoelectronics Applications*
13:10-14:30	**Lunch**		
	Session Chair: Dr. F.K Butt (UE, Faisalabad)	**Session Chair:** **Dr. Nadeem Nasir (NTU, Faisalabad)**	**Session Chair:** **Bin Amin (AUST, Abbotabad)**
14:30-14:50	**Abdul Khaliq Jan (SBBU, Dir)** *Nanomaterials as photocatalysts, RECENT ADVANCES IN g-C_3N_4*	**Rana Shahram Ali (University of Okara)** *Engineering of band gap by alteration of particle size of nano composite*	**Tanveer Hussain Bokhari (GCUF, Faisalabad)** *Synthesis and Characterization of*

		anode material	*NiCo2O4 based nanocomposites for energy storage purposes*
14:50-15:05	**Rabia Khatoon (LSBU, UK)** *Advanced Configuration of N-enriched Carbonized Tissue Paper as Free-Standing Interlayer for Lithium Sulfur Batteries at Wide Range Temperatures*	**M. Aqeel (UAF, Faisalabad)** *Synthesis and Characterization of CoS/V2O5/rGO-based nano-structured composites material for electrochemical energy storage device*	**M.A Javaid (NTU, Faisalabad)** *Synthesis and Characterization of Anti-microbial Polyester Resins for Organic Coatings with Bio-medical Potential*
15:05-15:20	**M. Saeed (GCUF, Faisalabad)** *Bi_2O_3-ZnO heterojunction; An effective solar-light-driven photocatalyst for degradation of organic pollutants*	**M. Inayyat ullah (GCUF, Faisalabad)** *Synthesis and characterization of $NiCo_2O_4$ based nanocomposites for energy storage applications*	**M. Shakil (IUB, Bahawalpur)** *Theoretical calculation of TMR of a magnetic tunnel junction designed using Co_2CrGe Heusler alloy*
15:20-15:35	**Rehan Gilani (BZU-Multan)** *Extensions of Stöber Method for the Preparation of Polymer Nanomaterials*	**Aisha Sethi (GCUF, Faisalabad)** *Reversed-Phase HPLC Method for quantification and identification of 5-Fluorouracil in Human and Rabbit Plasma Samples*	**Ahmed Waqar Aslam (IUB, Bahawalpur)** *First-principles investigation of structural, electronic, mechanical anisotropy, thermodynamic and optical properties of transition metal-based ternary TM5Si3C (TM = Mo, Nb, W, Ta) silicides of Nowotny phase*
15:35-15:50	**Hafiz Naeem ur Rehman (IUB, Bahawalpur)** *Optical and thermoelectrical behavior of*	**Shahid Anjum (GCUF, Faisalabad)** *Effect of Annealing on Thermoelectric Properties*	**M. Tayyab Hussain (UAF,**

	ZnO nanostructured layers coated with cobalt sulphide	*of Silver Sulfide Nanostructure*	**Faisalabad)** *Elemental Analysis of Doped Metallic Nanoparticles by Using Laser Induced Breakdown Spectroscopy*
15:50-16:05	**Sania Arif (UAF, Faisalabad)** *Enhanced photo-catalytic degradation of reactive dyes under UV/Visible light irradiation using efficient metal oxide nanocomposites*	**Amara Fatima (UAF, Faisalabad)** *Analysis of whole blood samples using Laser Induced Breakdown Spectroscopy coupled with machine learning*	**M. Zahid (UAF, Faisalabad)** *g-C_3N_4/graphene oxide/$SnFe_2O_4$ ternary composite for the effective sunlight-driven photocatalytic degradation of methylene blue*
18:30-20:30	**Cultural Night and Dinner**		
Day 3 **27 September, 2023**			
9:00-11:00	**Poster Session**		**Session Chair: Dr. Kashif Javaid (GCUF, Faisalabad)**
			09:00-09:15 **Amina Afzal (UET, Lahore)** *Tailoring Zeolite-Composite (ZC) Impregnated Nonporous Membranes for Potential Gas Separation and Antibacterial Performances*
			09:15-09:30 **Umber Kalsoom (UET, Lahore)** *Tailoring Mechanical Strength and Flexibility of PES Films with Metal Oxide Nanoparticles.*
			09:30-09:45

		Jawaria Z. Hashmi (UET, Lahore) *Influence of heat treatment on structural and optical characteristics of nano-crystalline Y-ZnO thin films*
		09:45-10:00 **Hamid Jamil (UET, Lahore)**
		10:00-10:15 **Aisha Nazir (UET, Lahore)** *Polymer Gel Electrolytes in Solid-State Dye-Sensitized Solar Cells: A Path to Stability and Efficiency*
		10:15-10:30 **M. Shoib (UET, Lahore)** *Tailoring Counter Electrode Performance with Graphene Oxide (GO) and Polyvinylpyrrolidone (PVP) for Enhanced Dye-Sensitized Solar Cells*
		10:30-10:45 **Zeshan Mustafa (LGU, Lahore)**
		10:45-11:00 **Z. Tanveer (NTU, Faisalabad)** *The enhancement of Physicochemical characterization of Zinc-Doped Nickel Oxide thin films through Chemical Vapor Deposition Method*
11:00-11:30	**Tea**	

	Hall 1 Session Chair: **Dr. Shahid Rafique (NSU, Islamabad)**
11:30-12:00	**N.M Butt (Preston University, Islamabad)** *The concept and importance of multidisciplinary BS degree in Nanotechnology and its positive results at national and international levels*
12:00-12:30	**Oswaldo Cadenas (LSBU, UK)** *Two ideas to shortcut scientific computations*
12:30-13:00	**M-A Hassan (UNCC, USA)** **TBA**
13:00-14:00	**Closing Ceremony**
14:00-15:00	**Lunch**

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MSNANO-23 (1)

Synthesis of Copper and Iron Doped ZnO Photocatalysts for Efficient Degradation of Reactive Dyes Under UV-Visible Light Irradiation

Muhammad Faheem[1], Ghulam Rasool Sani[1], Shagufta Riaz[3], Yasir Jamil[1], Yasir Javed[1] and Ayesha Younus[1,2]*

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Abstract

The worldwide contamination of the environment is probably regarded as one of the most serious issues that researchers will have to face during the current era. Toxic dyes are utilized extensively in different textile industries and to eliminate their contamination many methods are under consideration but photodegradation is one of the best strategies which is a chemically reliable, cost-effective, eco-friendly and highly efficient. Photodegradation encompasses the breaking down of larger organic compounds of dyes to smaller compounds like CO_2 and H_2O when dye solution is exposed to light. In this research work, Iron and copper doped ZnO nanoparticles (NPs)

were synthesized and their structural, morphological, chemical and electrical characteristics were studied by XRD, SEM, EDX, FTIR and IV characteristics, whereas UV-visible spectrometry was used to measure absorbance of dyes after different durations of time. XRD reveals wurtzite hexagonal structure with average size in range of 19-24 nm. The SEM analysis revealed that the nanoparticles consist of regular spherical shape with grain size observed in the range of 30–70 nm. The photocatalytic activity of two reactive dyes, Sandal Fix orange and Blue was assessed under UV-visible light at different pH values, i.e., pH 4, 7 and 12. Photodegradation efficiency of 91% was observed for both dyes at pH 12 in 120 and 105 min for blue and orange dye, respectively. The effect of pH, rate kinetics and other important parameters was investigated. It was observed that doped ZnO NPs exhibit greater photocatalytic efficiency than pure ZnO and

can be utilized as promising photocatalyst for degradation of industrial dyes. Both dyes exhibited higher photodegradation efficiency for the basic solution at pH=12.

MSNANO-23 (2)

Synthesis, Characterization and Compositional Study of Metal-Doped Copper Oxide Nanoparticles using Laser-Induced Breakdown Spectroscopy

Asad Akram[1], Khurrum Ali[1], Yasir Jamil[1], Rameeza[1] and Ayesha Younus[1,2]*

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Abstract

In this research work, the Co-precipitation method was utilized to synthesize undoped and cobalt-doped copper oxide (CuO) nanoparticles. These synthesized nanoparticles were characterized by XRD, SEM, UV-visible spectroscopy, FTIR and LIBS to determine their size, morphology, optical properties, functional groups and composition of doped and undoped nanoparticles. The monoclinic structure of CuO and Co-doped CuO nanoparticles was confirmed by XRD results. XRD revealed the crystallite size for doped and undoped NPs of CuO was in the range 15-30 nm. SEM images provided the information of the morphology of synthesized NPs that were spherical in shape. UV-Vis spectroscopy was used to get maximum absorption of samples. FTIR revealed the information about functional groups. For the LIBS analysis, the samples are atomized using a Nd:YAG laser working at its second harmonic (532 nm wavelength) capable of delving 250 mJ of energy, having a pulse duration and repetition rate of 5 ns and 10 Hz respectively. No trace of any impurity was detected in the samples and variation in the concentration was studied. Plasma temperature and electron number density of laser induced plasma were calculated to confirm local thermodynamic equilibrium (LTE) conditions using McWhirter criteria. Plasma temperature was between the range of 11300- 11500K. Electron number density was $1.24x10^{16}$ cm^3, $1.11x10^{16}$ cm^3 and $1.24x10^{16}$ cm^3 corresponding to undoped and Co-doped CuO samples. The application of principal component analysis, coupled

with LIBS spectra, presents a valuable approach for categorizing materials with changes in concentration.

MSNANO-23 (3)

Elemental Analysis of Doped Metallic Nanoparticles by Using Laser Induced Breakdown Spectroscopy

Aneeb Ullah[1], Ayesha Younus [1,2], Sania Arif[1], Hafeez Anwar[1], Yasir Jamil[1], M. Tayyab Iqbal[1]

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Abstract

Laser-induced breakdown-spectroscopy (LIBS) is a short pulsed laser which is centered on specimen to create plasma of high temperature. Due to quick sensitive optical-diagnostic, LIBS is currently being used to detect the specific species. In this experiment, a Q switched Nd-YAG laser of particular energy and specific wavelength used in order to record the spectra created by laser induced breakdown spectroscopy (LIBS) of sample. Numerous techniques have been described in the most recent decade, multi-beat LIBS, reverberation LIBS and different hyphenated procedures. Elemental analysis of nanoparticles directly analyzed by using Laser induced breakdown spectroscopy. The sample of different particle size take. By the aid of LIBS, plasma created on different samples of nanoparticles. The recorded elemental data of samples compared with National Institute of Standard and Technology. All the elements present in the synthesized NPs sample will be determine plasma temperature and electron number density calculated and local thermodynamics equilibrium condition verified. Calibration-free LIBS (CF-LIBS) was used to quantitatively analyze concentration of elements in a sample in local thermodynamic equilibrium conditions.

MSNANO-23 (4)

Measurement of propulsion parameters using aluminium and ferrites targets in external metallic cavities

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Abstract

Laser propulsion has been proved a blessing over chemical propulsion. Propulsion parameters include momentum coupling coefficient (C_m) and specific impulse (I_{sp}). In laser propulsion, optimizing the C_m is a crucial challenge. The cavities of metal with varying cavity aspect ratios were used. The pulsed Nd: YAG laser of 1064nm was focused on target, to generate plasma in a region enclosed by spherical cavities. To modify the Cm the generated plasma had been controlled by using spherical geometries. The measurement and calculation of parameters has been done using Aluminium and Ferrites propellants. To measure the parameters compound pendulum and light sensitive detectors were used. Cm, Isp were studied in this research work and we found that cavity having small aspect ratio (i.e. length to width ratio) shows and generate more thrust in comparison with the cavity having greater aspect ratio. We also found thrust produced by aluminium sample is greater than the thrust produced by ferrites sample. The calculated values of parameters have been compared at different fluence values with different cavity aspect ratios. Comparison made with external cavities and without cavities for propulsion parameters. All experiments were performed at room temperature and local thermodynamic equilibrium conditions.

MSNANO-23 (5)

Effect of dopants on thermoelectric properties of silver sulfide based nano-structures

Nimrah Tufail,

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Abstract

This study aimed to interlink several structural aspects of silver sulfide-based nanostructures with their thermoelectric properties. The silver sulfide-based nanostructures would be synthesized by hydrothermal method and post-sulfurization in a tube furnace. X-ray diffraction (XRD) will be used to study the crystallographic structural information, phase purity of and effect of post-sulfurization on crystallinity of the synthesized sample. Scanning electron microscopy technique will be applied to study synthesized nanostructures' morphology and grain sizes. Further structural analysis and study of the vibrational modes will be determined using Raman spectroscopy. The thermoelectric measurements will be carried out to see the thermoelectric efficiency, and the Seebeck and synthesized material's power factors will be calculated. The effect of dopants on structural parameters will be analyzed. The effect of dopants and post-sulfurization on the Seebeck coefficient and power factor would be investigated and would interlink with its structural parameters.

MSNANO-23 (6)

MODULATION OF THERMOELECTRIC PROPERTIES OF AlSe THIN FILMS BY POST-GROWTH ANNEALING IN Se ENVIRONMENT

Falak Naz

Department of physics, Government College University Faisalabad

Abstract

Concept of thermoelectric (TE) energy makes it distinctive because of reversible energy conversion, e.g. from thermal to electrical and vice-versa. Seebeck-Peltier effects are basis of all TE energy applications. Thermoelectricity has diversified scope of applications owing to

reversible energy conversion, which includes, electricity generation , heating and cooling etc. This research work will demonstrate quality growth of AlSe thin film by thermal evaporation method. Metal powders of Aluminum (A) and Selenium (Se) with 1:1 ratio will be evaporated from a tungsten boat in a thermal evaporation chamber on glass substrate. After growth, the film will be cut into pieces and post growth annealing in Se environment at different temperatures. The post-growth samples will be characterized using various techniques such as XRD, SEM, Raman spectroscopy, Hall measurements and Seebeck system. The effect of post growth annealing on structural, electrical and thermoelectric properties will be studied by calculating and comparing different performance parameter.

MSNANO-23 (7)

Epsilon-near-zero Response in Magnetron Sputtered Al-substituted Titanium Oxynitride Thin Films

Maria Khalil

Department of physics, University of Punjab, Lahore

Abstract

Epsilon-near-zero (ENZ) materials show vanishing permittivity in specific spectral regimes and have gained a lot of research interest because of their outstanding optical characteristics. The main objective of this study is the theoretical and experimental investigation of un-doped and doped Titanium oxide thin films in the quest for ENZ behavior. First-principles calculations based on the density functional theory (DFT) and experimental investigation were used to elucidate the effect of dopants on the electronic, structural, and optical response of samples. Pure TiO₂, N, and Al-doped TiO₂ thin films have been fabricated for the first time using a DC magnetron sputtering. The prepared films were subjected to different structural, morphological, and optical characterizations using X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), and spectroscopic ellipsometry (SE). ENZ behavior was successfully achieved experimentally at higher dopant concentrations, and it is in good agreement with our simulated results. The work presented in this study exhibited that

prepared oxynitrides thin films with ENZ response are suitable candidates for enhanced optoelectronic applications.

MSNANO-23 (8)

Study of Structural and Optical Properties of Carbon Nanostructures

MUMTAZ HUSSAIN

Department of physics, Government College University Faisalabad

Abstract

This R&D activity is made to introduce the facile and efficient approach to synthesize Carbon nanostructures by using cost effective, non toxic and environment friendly materials. Carbon nanostructure (CNs) has shown a considerable interest in a variety of applications, including biological sensing, photodynamic treatment, and nanofertilizers. Due to their exceptional electrical and optical characteristics in biomedical and photo catalytic applications, carbon nanostructure has received particular attention. Structural properties of synthesized carbon nanostructures will be studied by XRD and Raman analysis. Room temperature VSM measurements will be carried out to study magnetic properties and absorption properties will be studied by UV-Vis analysis.

MSNANO-23 (9)

ENGINEERING OF BAND GAP BY ALTERATION OF PARTICLE SIZE OF NANO COMPOSITE ANODE MATERIAL

Rana Shehram Ali

Department of physics, University of Okara

Abstract

Solid oxide fuel cell has got attention due to its salient features, fuel flexibility, high efficiency and environment friendly. To enhance the performance and efficiency the role of anode is very crucial because oxidation of fuel takes place at anode. In this research work, LaSrCrTiO3-δ

anode material has been synthesized by sol-gel method and characterized using various techniques. X-ray diffraction confirmed the orthorhombic structure of the prepared materials with crystallite size 21 nm. Scanning electron microscopy revealed porous structure and fabulous homogeneity with gran size roughly 500 nm. The band gap of anode material has been calculated, the lowest band gap is 2.52 eV for sample (d). The highest electrical conductivity has been measured 1.36 Scm-1 at 600°C for sample (d). These results show that LSCT is suitable material as anode for solid oxide fuel cell.

MSNANO-23 (10)

Redox active pyridine-3,5-di-carboxylate- and 1,2,3,4-cyclopentane tetra-carboxylate-based cobalt metal–organic frameworks for hybrid supercapacitors

Asma khizar

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Abstract

In the pursuit of developing superior energy storage devices, an integrated approach has been advocated to harness the desirable features of both batteries and supercapacitors, particularly their high energy density, and high-power density. Consequently, the emergence of hybrid supercapacitors has become a subject of increasing interest, as they offer the potential to merge the complementary attributes of these two technologies into a single device, thereby surpassing the limitations of conventional energy storage systems. In this context the Metal–Organic Frameworks (MOFs), consisting of metal centers and organic linkers, have emerged as highly trending materials for energy storage by virtue of their high porosity. Here, we investigate the electrochemical performance of cobalt-pyridine-3,5-di-carboxylate-MOF (Co-PDC-MOF) and cobalt-1,2,3,4-cyclopentane tetra-carboxylate-MOF (Co-CPTC-MOF). In the setup involving the analysis of Co-PDC-MOF and Co-CPTC-MOF materials, a configuration comprising three electrodes was utilized. Drawing upon the promising initial properties of CPTC, a battery device was fabricated, comprising Co-CPTC-MOF, and activated carbon (AC) electrodes. Retaining a reversible capacity of 97% the device showcased impressive energy and power density of 20.7

W h g^{-1} and 2608.5 W kg^{-1}, respectively. Dunn\'s model was employed, to gain deeper insights into the capacitive and diffusive contributions of the device.

MSNANO-23 (11)

METAL-ORGANIC FRAMEWORKS FOR SUPERCAPACITOR-BATTERY HYBRIDS

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Abstract

In modern times, energy consumption, depletion of conventional sources and climate changes are the major concerns that needs to pay real attention. In order to resolve energy crisis for upcoming energy intensive era, researchers are trying to develop sustainable storage devices and renewable energy sources. Today’s electrically driven world raises the demand of both high power and energy density in energy storage systems. The two forefront energy storage technologies i.e., supercapacitors and batteries are currently fulfilling the energy storage exigency. However, hybrid supercapacitor-batteries have tendency to conjoin the features of both in a single device for efficient and enhanced outcomes. Electrode material selection is a crucial step before fabricating an energy storage device because the outcomes of the device rely upon the materials utilized. Different materials and their composites are used as electrode (anode and cathode) materials in supercapacitor-battery hybrids.Metal organic frameworks (MOFs) are kind of hybrid materials based on organic (linker) and inorganic (metal nodes) constituents. Relative to the traditional 3D MOFs, the layered coordination polymers (2D MOFs) show some distinct and prominent features such as spatial connectivity, enhanced conductivity, tunable structure, and more exposed area etc. These 2D conductive MOFs are potential materials for conventional applications.

MSNANO-23 (12)

Binary and ternary mixed metal oxide thin films fabrication by AACVD for optical and Solar water splitting

Dr. Rabia Naeem

Department of Chemistry, Government College University Lahore

Abstract

This work investigates the interest of solar water splitting as a auspicious method for hydrogen production. the production of hydrogen. Therefore, fabrication of efficient photoelectrode is vital to attain better performance cells. Aerosol-assisted chemical vapor deposition (AACVD) is describing as a versatile fabrication technique for the manifestation of thin films in terms of their homogeneity and uniformity. From this point of view, we explain the AACVD method and the effect of the fabrication factors like precursor, temperature, solvent, deposition time, presence and absence of electric field on PEC water splitting. The better morphological and optical properties of films fabricated by AACVD method have been confirmed to enhance the proficiency of the PEC water splitting process.

MSNANO-23 (13)

Effect of Annealing on Thermoelectric Properties of Silver Sulfide Nanostructure

Shahid Anjum

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Abstract

In this research work we explores the structural intricacies influencing the thermoelectric properties of silver sulfide nanostructures, achieved by varying silver and sulfur concentrations through thermal evaporation. Assessment through Raman spectroscopy, X-ray diffraction (XRD), and scanning electron microscopy (SEM) reveals crucial structural and electrical attributes. The hydrothermal process followed by sulfurization at varying temperatures, yields

high-purity polycrystalline silver sulfide nanostructures. These structures are then used to create pellets for thermoelectric analysis, considering changes in sulfurization temperature and their impact on thermoelectric data. Our method provides a rapid route to produce thermoelectric silver sulfide nanoparticles with optimized properties. Precursors include silver nitrate and sodium thiosulfate, and experimental tools encompass electronic ovens, balances, beakers, magnetic stirrers, autoclaves, and filter paper. Overall, this approach offers a promising path to enhance the quality and thermoelectric performance of silver sulfide nanostructures, primarily through annealing.

MSNANO-23 (14)

First-principles investigation of structural, electronic, mechanical anisotropy, thermodynamic and optical properties of transition metal-based ternary TM5Si3C (TM = Mo, Nb, W, Ta) silicides of Nowotny phase

AHMAD WAQAR ASLAM

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Abstract

In this work, the structural, mechanical, thermodynamic, and opto-electronic properties of TM₅Si₃C (TM = Mo, Nb, W, Ta) silicides are examined using first-principles calculations. All studied silicides fulfil the structural and mechanical stability criteria. Computed mechanical properties reveal the ductile nature of Mo₅Si₃C, Nb₅Si₃C, and W₅Si₃C silicides, while Ta₅Si₃C silicide is brittle in character. Elastic anisotropy plots, including 2D and 3D, show highly anisotropic behaviour. The studied electronic and dielectric properties validate the conductive nature of all these silicides. All silicides in the visible region have an average reflectivity of 46%, making them ideal for coatings to reduce solar heat radiation. Debye temperature, melting point, thermal conductivity, and grneisen constant have also been investigated in current work. Thermodynamic

properties are calculated at different pressure and temperature including bulk modulus (), volume (), thermal expansion coefficient (), debye temperature (), and lattice heat capacity (). The probed results of TM₅Si₃C ternary silicides demonstrate their viability as solar reflectors and optoelectronic devices. Our findings also provide a gateway for exploring new ternary silicides and can act as an efficient, cost-effective guide for experimentalists.

MSNANO-23 (15)

Theoretical investigations of the structural, elastic, electronic, magnetic and thermoelectric properties of MRh2O4 (M = Mg, Mn, Cd) spinels.

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Abstract

First-principles calculations have been performed to investigate the structural, mechanical, electronic, magnetic and thermoelectric properties of MRh₂O₄ (M = Mg, Mn, Cd) spinel oxides. Calculations reveal that all oxides are structurally and mechanically stable. Elastomechanical results provide that the CdRh₂O₄ is ductile, MnRh₂O₄ is brittle, while MgRh₂O₄ lies on ductile/brittle borderline. The high bulk modulus and Young's modulus of MnRh₂O₄ensure its ability to resist volume change and plastic deformation, showing the material's suitability for industrial applications. MnRh₂O₄ spinel oxide bears the highest values of Debye temperature (T_D = 634.4 K) and melting temperature (T_M = 3530.4 K) among the MRh₂O₄ (M = Mg, Mn, Cd) oxides. Band structure calculations and density of states (DOS) spectra indicate the p-type semiconducting nature of MRh₂O₄ (M = Mg, Mn, Cd). Spin-polarized electronic structure of CdRh₂O₄ oxide is found to exhibit 100 % spin-polarization, while MgRh₂O₄ and MnRh₂O₄ oxides show 0.12 % and 0.29 % spin-polarization,

respectively. MnRh₂O₄ is found to have the highest saturation magnetization (172 emu/g) and total magnetic moment (9.99 μ_B/f.u.). Thermoelectric properties (thermal and electrical conductivities, Seebeck coefficient (S), figure-of-merit (ZT), Hall coefficient (R_H) and power factor) as a function of temperature are also reported. Based on results studying thermoelectric behavior, MRh₂O₄ (M = Mg, Mn, Cd) oxides are proposed for applications as novel thermoelectric materials.

MSNANO-23 (16)

Structural, morphological and magnetic properties of M-type hexaferrites

Ghulam Asgha

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Abstract

Simultaneous occurrence of more than one ferroic order in a material is of great importance from an advanced technological point of view. M-type hexaferrites possess multiferroic order. Barium hexaferrite was synthesized by the oxide powder metallurgy (wet/dry) route for multiferroic applications. Powder and pallets of prepared samples were annealed/sintered in the temperature range between (800-1200) ℃ for 2 hours in air to Improve phase purity of samples. Suitable heat treatment and grain growth inhibitors (SiO2 and CaO) were used to control and optimize the microstructure of prepared particles. Properties of multi-ferroic oxide ceramics (ferrites) were tailored by doping La. Samples were characterized for thermal, phase analysis, surface morphology, chemical, magnetic and electrical analysis using simultaneous thermal analyzer (STA), X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), magnetometer and ferroelectric tester. Indexed XRD patterns revealed that single phase hexaferrite was obtained at 1000 ℃. Unit cell volume and X-ray density obtained from XRD at different temperatures was in range of (712-703) Å³ and (5.18-5.25) g/cm3 respectively. It was found from scanning electron microscopic analysis that all samples had grains with square, hexagonal, and elongated shapes. STA spectra showed two endothermic peaks at 770 ℃ and 936 ℃. Weight loss at these temperatures was 7 percent and 10 percent

respectively. From P-E loops, it was observed that low concentration of La is favorable for electric polarization. It was observed from MH loop that saturation magnetization and coercivity increases with increases temperature and after Curie temperature, these values started decreasing.

MSNANO-23 (17)

Structural, optoelectronic, elastomechanical and thermodynamic properties of Na2Fe2S2O oxy-chalcogenide: A computational study

Muhammad Haseeb

Institute of Physics

Abstract

The materials that possess narrow band-gap have got great attention in the field of optoelectronics for a number of applications like as infrared radiation detection. In this study, the structural, optoelectronic, elastomechanical, and thermodynamic properties of Na₂Fe₂S₂O oxy-chalcogenide have been studied using first-principles method. Within the framework of density functional theory Wien2k code is used to perform all theoretical calculations. Due to the acceptance of all stability conditions, Na₂Fe₂S₂O oxy-chalcogenide is mechanically stable. Electronic properties illustrate that electron correlations in the Fe-d bands promote a transition of Na₂Fe₂S₂O from magnetic metallic or half-metallic states to the antiferromagnetic Mott-insulating state. Optical properties as well as DOS data indicate that the examined quaternary oxy-chalcogenide, Na₂Fe₂S₂O, has a narrow band gap (less than 1 eV, closed results with the literature value). Optical spectra display that absorption lies in the visible as well as in the UV region of the radiation. As a result, it looks to have probable applications in optoelectronics. Anisotropy in all moduli (Young's modulus, Shear modulus, Bulk modulus, Poisson's ratio) is calculated and presented with 2D and 3D visualization. 2D and 3D spectra of Na₂Fe₂S₂O oxy-chalcogenide show anisotropic nature in (010) and (100) planes however isotropic in (001) plane. Furthermore, pressure and

temperature-dependent thermodynamic parameters for the studied compound are also computed using quasi-harmonic Debye approximation.

MSNANO-23 (18)

First-principles study on the structural, mechanical, electronic structure, thermal and thermophysical properties of XS (X = Ge, Sn, Pb) monochalcogenides

Muhammad Amir Rafiq

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Abstract

First-principles calculations of XS (X = Ge, Sn, Pb) monochalcogenides are performed for four different crystallographic arrangements such as cubic (SG# 225), orthorhombic (SG# 62), hexagonal (SG# 186) and trigonal (SG# 160). Among these crystalline phases, orthorhombic GeS, orthorhombic SnS and trigonal PbS monochalcogenides are found to have the most stable crystal structures. Mechanical properties of orthorhombic GeS, orthorhombic SnS and trigonal PbS monochalcogenides has been calculated which reveals that the orthorhombic XS (X = Ge, Sn) monochalcogenides fulfill the Born stability conditions, while trigonal PbS does not meet Born stability criteria. Calculated Poisson's ratio (ν) and Pugh's ratio indicate the brittle nature of orthorhombic GeS and ductile nature of orthorhombic SnS. Poisson's ratio reflects that orthorhombic SnS exhibits metallic bonding while orthorhombic GeS has non-ionic bonding. Furthermore, mechanical anisotropy is found in ortho-GeS and ortho-SnS monochalcogenides. The vibrational response of studied sulfides has also been investigated using Debye temperature. Electronic band structure calculations reveal that the XS (X = Ge, Sn) monochalcogenides exhibit p-type semiconducting nature. Orthorhombic GeS exhibit a direct band gap E_g = 1.14 eV, while orthorhombic SnS has indirect Eg = 1.149 eV. The possible applications based on mechanical, electronic, and thermal physical properties have been outlined.

MSNANO-23 (19)

A Comparative Study of Different Physical Properties of Nowotny Phase TM5Si3C (TM = Nb, Mo) Ternary Silicides

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Abstract

The structural, electronic, mechanical, optical and thermodynamic properties of Nowotny phase ternary silicides Nb₅Si₃C and Mo₅Si₃C are calculated. WIEN2k package based on density functional theory is utilized to study different physical properties. Theoretical calculations are carried out through generalized gradient approximation (GGA). A comprehensive analysis of the predicted results demonstrate the similar but not identical behavior of both ternary compounds. TM₅Si₃C (TM = Nb, Mo) silicides reveal hexagonal crystal structure and possess space group P6₃/mcm (space group no. 193). There are 4 non-equivalent sites for both ternary compounds. Structural optimization demonstrates the stability of a structure along with the minimum energy. k-sampling briefly explain the discretizing of Brillouin zone into different k-points. All the properties are calculated at the specific k-points 1400 (101012). Plots of band structure and density of states (DOS) show that the investigated compounds are metallic in nature. Orbital resolved density of states demonstrate that TM1-d and TM2-d have major contribution at fermi level. Furthermore, these silicides fulfill the Born's mechanical stability criteria. The results of mechanical properties (Cauchy pressure, Pugh's ratio and Poisson's ratio) illustrate that these compounds have ductile nature and ionic bonding exist in both compounds. Bulk modulus, Young's modulus and shear modulus describe the compressibility, stiffness and deformation resistance of a compound. Due to high melting point Nb₅Si₃C and Mo₅Si₃C are suitable candidates for high temperature materials. Negative value of dielectric function confirms the metallic nature of compounds while indicates the absorption and energy loss phenomena. Intraband transitions near 0.0 eV in

optical conductivity validate the metallic behavior of ternary silicides. Both silicides exhibit their peaks in ultraviolet region. When high-energy electrons pass through the metal, the energy loss peak appears not only at the plasmon frequency of the metal film but also at lower frequencies. The occurrence of plasma resonance is demonstrated by high energy peaks in electron energy loss function curves indicating maximum energy absorption. Thermodynamic properties are explored under the broad range of temperature (0-1000 K) and pressure (0-80 GPa). These compounds are thermally stable due to the high value of Debye temperature and specific heat capacity.

MSNANO-23 (20)

Green Metal Nanoparticles: An Eco-Friendly Approach for Advancing Cancer Treatment"

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Abstract

Despite significant advancements in cancer research, understanding, and treatment, the global incidence of cancer continues to rise, maintaining its status as a leading cause of death. Early detection and screening play pivotal roles in the fight against cancer, facilitating more effective therapies and reducing mortality rates associated with the disease. Various treatment modalities exist for combating cancer, including surgery, chemotherapy, immunotherapy, phototherapy, radiation therapy, and targeted therapy, among others. While conventional chemotherapy has been successful in treating several types of cancer, it presents several limitations, such as low bioavailability, high dosage requirements, drug resistance, adverse side effects, and a lack of precision in targeting tumor tissue. In contrast, targeted therapy utilizes therapeutic agents designed to specifically target genes and proteins critical for the growth and survival of cancerous cells. These agents are administered to solid tumors through the bloodstream, often via the injection of micro and nanoparticles. One promising approach involves the precise delivery of cytotoxic drugs to malignant cells using environmentally friendly biogenic gold (AuNPs) and silver-based nanoparticles (AgNPs). Despite its potential, this strategy has not been extensively developed or explored until now. The study provides an up-to-date overview of the latest

advancements in green biological synthesis methods for producing AuNPs and AgNPs and their potential applications in cancer treatment.

Key words: Nanoparticles, green synthesis, cancer treatment, Metallic Nanoparticles

MSNANO-23 (21)

First-principles Calculations of ScMC2 (M = Fe, Co, Ni, Cu) Ternary Carbides: A Suitable Candidate for Shielding Purpose

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Abstract

Physical properties of scandium-based ternary carbides ScMC₂ (M = Fe, Co, Ni, Cu) have been investigated using first-principles calculations. The Wien2k code based on Density Functional Theory (DFT) is employed for these calculations. The study confirms that ScMC₂ carbides meet the thermodynamic, mechanical and thermal stability criteria. Various properties including thermophysical, mechanical anisotropy and optical characteristics are reported for the first time. The optimization data reveal ScCuC₂ as the most stable structure. Carbon-carbon (C-C) bond lengths vary among the studied compounds. Stiffness constants and elastic moduli are calculated and compared with previously reported results. Poisson's and Pugh's ratios suggest ductile nature of ScMC₂ (M = Fe, Co, Ni) compounds, while ScCuC₂ bears brittle behavior. The thermal shock resistance ranking is ScNiC₂ > ScCoC₂ > ScCuC₂ > ScFeC₂. These carbides also show improved thermal properties, machinability, rigidity, melting point, resistance to bond elongation and torsional deformations. DOS (density of states) spectra indicate metallic behavior of ScMC₂ (M = Fe, Co, Ni, Cu) carbides with electronic states decreasing progressively at the Fermi level (E_F) with different transition metals. Optical properties reveal anisotropy in ScMC₂ carbides up to 30 eV and reflectance spectra suggest that

ScCoC₂ is the most suitable candidate for shielding and solar heating mitigation among the studied compounds.

MSNANO-23 (22)

Strained Mechanical Analysis of Carbon Nanotube Using Molecular Dynamics Simulations

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Abstract

Carbon nanotubes (CNTs) have emerged as one of the most capable and intriguing materials in recent decades having extraordinary mechanical properties and resourceful applications. This study employs equilibrium molecular dynamics (EMD) simulations to explore the structural and mechanical properties of armchair, chiral, and semiconducting and metallic zigzag SWCNTs under varying temperature T(K), compressive and tensile strains ±γ(%). These configurations are simulated at varying T= 300K, 500K and 700K, revealing intricate insights into their behavior when subjected to combined compressive and tensile strains. New simulations show that the buckling and breaking processes of single-walled CNTs (SWCNTs) with varying nanotube length L (A), T(K) and ±γ(%). Radial Distribution Function (RDF) test is performed to investigate the mechanical properties of SWCNTs and focusing on the potential benefits in various fields. The main objective of this study is to uncover the mechanical responses from different chirality's of SWCNTs, elucidating variations in tensile strength in terms of temperature. Stress-strain analyses reveals that (12,0) have superior tensile strength compared to (8,8) and (8,0) whereas (8,4) having lowest tensile strength. Leveraging these findings, nanotube materials can be tailor-engineered for specific mechanical properties, thus opening doors to innovative applications across diverse domains.

MSNANO-23 (23)

Radiosensitization Effects of Gold Nanoparticles in Proton Treatment

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Abstract

Ionizing radiations of proton have significant effect of cellular response of breakage and damage of DNA double strand. Targeted radiotherapy with gold nanoparticles (AuNPs) enhanced the efficiency of DNA damage without affecting the surrounding normal cells. The AuNPs increased the radiosensitivity of tumor cells. In this study dose enhancement and energy depositions has been investigated by the different sizes of AuNPs at different energies using proton beam. The radiosensitziation characteristics of AuNPs were investigated in a single cell irradiated with monoenergetic beams of protons of various energies using TOPAS-nBio, an advance toolkit of TOPAS. In Monte Carlo (MC) track structure TOPAS-nBio, both direct and indirect effects have been studied to calculate double strand break (DSB) and single strand break (SSB). A mixed-physics approach was taken into account for accurate modeling of charged particle interactions in different regions of simulation model. A single spherical cell with a detailed DNA structure was simulated under various conditions including different sizes and concentrations of gold nanoparticles, biodistribution, and proton energies.

MSNANO-23 (24)

Structural and optical characterization of ZnS and (Co, Fe) co-doped ZnS nanoparticles

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Abstract

In this work, the structural and optical properties of pure ZnS and Fe/Co co-doped ZnS nanoparticles are presented. XRD pattern revealed the single-phase cubic structure for prepared samples. SEM technique was employed to observe the morphology of samples. The absorption spectra illustrated the decrease in optical energy band gap with Fe/Co co-doping in ZnS. The values of refractive index confirmed the direct relation with dopant. PL spectra demonstrated the emission peaks which are related to native defects. This work enhances the understanding of structural and optical properties of Fe/Co co-doped ZnS nanocrystals for various applications such as solar cells, and ceramics.

MSNANO-23 (25)

Bi2O3/WO3 Heterostructure as Efficient Solar Driven Photocatalyst

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Abstract

The industrial waste water is always matter of challenge polluting the environment and ultimately causing a hazardous effect to human beings and various other species. For the elimination of these pollutants, in this study, we synthesized Bi₂O₃ nanoparticles and Bi₂O₃/WO₃ heterostructure and investigated their photocatalytic activity for the degradation of methylene blue (MB) under solar light irradiation. A chemical co-precipitation approach was used to synthesize the nanoparticles (NPs) and these NPs were characterized by various analytical techniques, including X-ray

diffraction (XRD), Scanning-electron-microscopy (SEM), Fourier-Transform-Infrared Radiation (FTIR) and UV-Vis. Spectroscopy. The result of this study revealed that the Bi₂O₃/WO₃ nanocomposite exhibited significantly enhanced photocatalytic activity compared to pure Bi₂O₃. Under sunlight irradiation, the Bi₂O₃/WO₃ nanocomposite degraded 79.4% of MB in 210 min, while pure Bi₂O₃only degraded 58.8% of the MB in the same time period. The enhanced photocatalytic performance of the nanocomposite can be attributed to the synergistic action between Bi₂O₃and WO₃, which enhances the production of reactive oxygen species (ROS) and the efficiency of charge separation, thus promoting the degradation of MB. The results of this study highlight the potential of Bi₂O₃/WO₃ nanocomposites as promising materials for environmental remediation applications, particularly for the efficient removal of organic pollutants from wastewater under solar irradiation.

Key Words: heterostructure; ROS; nanocomposite; photocatalysis; wastewater.

MSNANO-23 (26)

Effect of Fe co-doping on the structural and optical properties of Co:ZnO nanoparticles

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Abstract

Fe (x = 0.00, 0.05, 0.10 and 0.15) co-doped with Zn _{0.8} Co _{0.2} O (Co:ZnO) nanoparticles were prepared using a simple hydrothermal method. The effect of Fe on structural morphological and optical properties was investigated with the help of X-ray Diffraction (XRD) pattern, Scanning Electron Microscopes (SEM), UV-Visible Spectroscopy (UV-Vis) and Photoluminescence (PL) respectively. XRD pattern proved the formation of wurtzite hexagonal structure for the Fe (x = 0.00, 0.05, 0.10 and 0.15) co-doped Co:ZnO samples. The average particle size of the Co:ZnO samples were calculated in the range of 19-32nm from the XRD results. Blue shift of the absorption band was observed and diminution in

the optical transmittance behavior was estimated for the Fe co-doped Co:ZnO samples in the UV–Visible analysis. The bandgap value was also found decrement with increment of metal (Fe) dopant concentration. Photoluminescence (PL) emission spectra exhibit first decrease then increase in intensity and shift towards high frequency in the visible region and UV region for the Fe co-doped Co:ZnO samples. These observations indicate the possibility of tuning structural and optical properties of metal (Fe, Co) doped ZnO with various dopant concentrations of iron and will have great potential to find application in optoelectronic devices.

MSNANO-23 (27)

Influence of distances between lens to Al sample surface on laser-induced breakdown spectroscopy

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Abstract

Laser-induced breakdown spectroscopy (LIBS) is a very promising spectral analysis technique for detecting element composition. It is favored by researchers because of its many advantages, such as real-time analysis, multi-elemental analysis, simple or no sample preparation requirements, and remote analysis. In recent years, this technology has been widely used in many fields. However, the problem of low detection sensitivity of LIBS technology is becoming more and more obvious. Therefore, improving spectral intensity has become the focus of researchers. The expansion dynamics of the plasma plume depend on the distance between the target surface and the focal point. In this work, a significant influence of lens-to-sample distance on the signal of laser-induced breakdown spectroscopy is represented. Laser-induced Al plasma by using an Nd: YAG nanosecond laser at different distances between the lens and sample surface was investigated. The results indicated that the intensity of Al (I) 394.4, 396.2 nm line first rose and then dropped with the increase of lens-to-sample distance at fixed laser energy. The research has significance for enhancing the plasma signal which led to improved LIBS sensitivity.

MSNANO-23 (28)

SYTHESIS AND ELECTROCHROMIC EVALUTION OF GRAPHENE QUANTAM DOTS/POLYVINYL ALCOHOL

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Abstract

Graphene quantum dots proved emerging candidates in the field of material sciences because of their potential applications in different fields. Therefore, facile, economical, and eco-friendly synthetic approaches were carried out in which indigenous and readily available coal and graphene oxide (GO) was used as precursor material. Hydrothermal treatment method under a top-down approach was successfully developed to synthesize coal-derived graphene quantum dots (C-GQDs) and graphene oxide derived (G-GQDs). Synthesized C-GQDs and G-GQDs were seen under an ultraviolet (UV) lamp of 365 nm, characterized by UV-vis and Fourier transform infrared spectroscopy (FTIR) spectroscopy. To, improve the optical transparency, mechanical stability and reduce agglomeration of GQDs composite film synthesized by solution casting method. In this method polymer polyvinyl Alcohol (PVA) is provided as matrix and obtained composite film C-GQDs/PVA and G-GQDs/PVA. Synthesized composite films seen under UV lamp 365 nm and further characterized by FT-IR, thermogravimetric analysis (TGA), and photoluminescence (pL) spectroscopy.

MSNANO-23 (29)

Tailoring Mechanical Strength and Flexibility of PES Films with Metal Oxide Nanoparticles.

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Abstract

Loading metallic oxide nanoparticles, specifically zinc oxide (ZnO) and copper oxide (CuO), into a Polyethersulfone (PES) matrix has a significant impact on the properties of the composite materials. Enhancements in the physical and mechanical properties of PES depend on the type, size, and concentration of the nanofillers added to the PES matrix. The solution casting method is employed to synthesize films that blend PES with metallic oxide nanoparticles. Field emission electron microscopy (FESEM) reveals rod-like, semi-spherical, and rhombus-shaped structures of ZnO and CuO nanoparticles, which result in improved structural and mechanical properties. The interaction between nanoparticles (NPs) and PES induces structural strain, resulting in improved mechanical properties in the PES-loaded films. The tensile strength has increased from 2.63 MPa to 5.65 MPa with the addition of ZnO nanoparticles, while the Young's modulus has also improved from 8.92 MPa to 10.02 MPa. Notably, a more significant increase in mechanical properties is observed in the case of CuO nanoparticle-loaded PES blended films.

MSNANO-23 (30)

Development of Novel Deep Learning-Based Segmentation Models using MRI images for Low-Grade Glioma Brain Tumor segmentation

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Abstract

Among brain tumors, low-grade gliomas (LGG) tumor segmentation presents a unique challenge due to their infiltrative and heterogeneous nature. Traditional segmentation methods often struggle to address the complexities of these tumors. Recent advances in deep learning have revolutionized medical image analysis, offering promising solutions for improved accuracy and efficiency in tumor segmentation tasks. However accurate LGG tumor segmentation is still a challenge due to its heterogeneity, infiltration, variability and variation in size and location in the brain. In this context, this study focuses on the development and evaluation of a novel deep learning-based segmentation model tailored specifically for LGG brain tumors. Unet-based architecture with attention mechanisms and skip connections has been trained to improve the efficiency of conventional deep learning-based segmentation models. Different image data augmentation techniques have also been employed to handle the overfitting and dataset scarcity issues. LGG brain tumor publicly available MRI imaging dataset from The Cancer Imaging Archive (TCIA) and The Cancer Genomics Atlas (TCGA) together with Fluid-attenuation inversion recovery (FLAIR) segmentation masks annotated by medical experts have been used to train this designed segmentation model by using Adamax and dice loss as optimizer and loss respectively and Colab resources. Training metrics of accuracy, intersection over union (IOU) coefficient and Dice coefficient calculated during the training phase are 0.98, 0.89 and 0.92, respectively, while these metrics for validation datasets are found to be 0.97, 0.81 and 0.88 respectively. These outcomes indicate the efficiency of the model architecture and training process for correctly segmenting the tumors in brain MRI images.
Keywords: low-grade glioma brain tumor LGG, U-Net, Attention U-Net, IOU, Dice

MSNANO-23 (31)

Development Of Technecium-99m Labeled Nanoparticles Loaded With Antimicrobial Agent As Spect Imaging Agent

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Abstract

Radiotherapy is an innovative, targeted therapy that drives down high drug concentrations by improving the pharmacokinetics of the drug. This leads to better diagnosis and treatment outcomes. As a novel imaging platform for tumor targeting, moxifloxacin-chitosan nanoparticles as a drug delivery system may be manufactured using an ionic gelation process. This technology also serves as a potential drug delivery system. Chitosan nanoparticles have received a lot of interest especially due to their al-encompassing antibacterial properties. The purpose of this research was to develop radiopharmaceuticals that are non-toxic to the human body, have greater imaging efficacy, better accumulation at the targeted location, improved bioavailability, and increased exposure. Chitosan is a substance that is well-suited for usage in medical applications because of a variety of its biological characteristics. Biodegradability, non-toxicity, anti-fungal actions, faster wound healing, and immunologic activation are some of these qualities. In this study, 103nm-sized chitosan nanoparticles exhibit a zeta potential of 3.3± 0.4 mV, a high moxifloxacin loading efficiency of 99.3%, and drug entrapment efficacy of 85.66%. Moxifloxacin-chitosan nanoparticles were radiolabeled with technetium-99m using stannous chloride as a reducing agent and a pH of 6. The radionuclide was eluted using a fission-based 99Mo/99mTc generator that was created locally, and imaging was done using single-photon emission computed tomography (SPECT). The quality control experiments suggest that Moxifloxacin-loaded chitosan nanoparticles with technetium-99m had labeling effectiveness of more than 75%. Radiochemical yield was examined using instant thin layer chromatography (ITLC) methods. Rats that had been given an infection with Escherichia coli (E.coli) were used to study the biodistribution and infected specificity of the 99mTc radiotracer. Following injection of 99mTc-moxifloxacin-chitosan nanoparticles, renal uptake was 4.46± 0.66% at 30 minutes and

1.77 ± 0.07 at 6 hours, while liver uptake was 2.66 ± 0.16% at 30 minutes and 0.62 ± 0.06 at 6 hours. On the basis of the observed findings, it can be inferred that the newly created 99mTc-moxifloxacin chitosan nanoparticles could be employed as an effective diagnostic agent for deep-seated bacterial infections.

MSNANO-23 (32)

Facile synthesis of CuAl2O4/rGO nanocomposite via the hydrothermal method for supercapacitor applications

Shahzaib Khan

Department of Chemistry, Government College University Faisalabad

Abstract

Transition metal-based spinel oxides are fascinating supercapacitor electrode materials due to their good specific capacitance (Cs) and cost-effectiveness. However, the spinel materials show poor cycling stability due to their limited surface area. This issue was reduced by using carbon-based electrode materials such as rGO, which enhances the electroactive surface area and leads to an improvement in the number of reactive sites. In this research, a simple hydrothermal approach was utilized to synthesize the CuAl2O4/rGO (CAO/rGO) nanocomposite. It is successively characterized by different analytical techniques to study the physiochemical properties of the synthesized materials. Additionally, the potential of the materials as the electrode was determined with a three-electrode configuration by utilising different electrochemical tools that were performed to assess the characteristics of the electrode material. The synthesized nanocomposite exhibits a magnificent specific capacitance (Cs) of 1206.14 F/g at 1 A/g while demonstrating specific energy (Ed) of 34.83 Wh kg−1 and specific power (Pd) of 228 W kg−1 which is higher than individuals and also shows high retention capacitance value of 93.36% after 8000th charge/discharge (GCD) cycles. The symmetric behavior of the fabricated electrode is also determined with two electrode systems exhibiting the specific energy and specific capacitance of 16.54 Wh kg−1 and 601.91 F/g, correspondingly. This study demonstrates that incorporating rGO into CuAl2O4 nanoarray improves energy storage performance and it has the potential to work in other energy storage devices.

MSNANO-23 (33)

Influence of heat treatment on structural and optical characteristics of nano-crystalline Y-ZnO thin films

Jaweria Zartaj Hashmi

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Abstract

Thin films of yttrium doped zinc oxide have been deposited successfully on borosilicate glass substrates using pulsed laser deposition. The as deposited films are annealed at 400 °C and 600 °C. Influence of annealing is examined for undoped and Yttrium doped ZnO by collecting data from XRD, UV-vis spectroscopy and Photoluminescence spectroscopy. XRD spectrum indicate polycrystalline growth which improves with annealing temperature. The structural defects created by deposition parameters or dopant are clearly affected by heat treatment. The structural variations also correspond to optical characteristics like absorbance, band gap and luminescence. It is concluded that the properties of rare earth doped zinc oxide can be significantly modified by applying a heat treatment that can provide sufficient thermal energy for the adatoms to re-arrange themselves in their favorable spots. Thus, structural defects can be controlled, and the material can be used in device fabrication.

MSNANO-23 (34)

Polymer Gel Electrolytes in Solid-State Dye-Sensitized Solar Cells: A Path to Stability and Efficiency"

Aisha Nazir

Department of Physics, UET Lahore

Abstract

The indispensable role of fossil fuels in satisfying 80% of global energy demand is diminishing rapidly and concurrently exacerbating carbon dioxide (CO2) emissions. Consequently, there is a

concerted worldwide effort to explore cleaner energy alternatives, with renewable energy emerging as a highly promising candidate. Nonetheless, challenges are prevalent in harnessing solar energy efficiently. Consequently, attention is now redirected toward 3rd Generation photovoltaic devices, specifically Dye-Sensitized Solar Cells (DSSCs), which offer a cost-effective solution and exhibit the highest level of electricity conversion efficiency. The significance of electrolytes within DSSCs cannot be overstated, as they facilitate charge transport and exert a substantial influence on the stability and performance of these devices. While liquid electrolytes have proven efficient, they are susceptible to issues such as leakage and evaporation. In recent years, gel-based polymer electrolytes (PGEs) have emerged as a highly promising alternative, effectively addressing the leakage problem. This research endeavor seeks to harness the potential of gel-based polymer electrolytes to achieve elevated levels of conversion efficiency and enhance the overall energy conversion capabilities of DSSCs.

MSNANO-23 (35)

Polymer Gel Electrolytes in Solid-State Dye-Sensitized Solar Cells: A Path to Stability and Efficiency"

Aisha Nazir

Department of Physics, UET Lahore

Abstract

The indispensable role of fossil fuels in satisfying 80% of global energy demand is diminishing rapidly and concurrently exacerbating carbon dioxide (CO2) emissions. Consequently, there is a concerted worldwide effort to explore cleaner energy alternatives, with renewable energy emerging as a highly promising candidate. Nonetheless, challenges are prevalent in harnessing solar energy efficiently. Consequently, attention is now redirected toward 3rd Generation photovoltaic devices, specifically Dye-Sensitized Solar Cells (DSSCs), which offer a cost-effective solution and exhibit the highest level of electricity conversion efficiency. The significance of electrolytes within DSSCs cannot be overstated, as they facilitate charge transport and exert a substantial influence on the stability and performance of these devices. While liquid electrolytes have proven efficient, they are susceptible to issues such as leakage and evaporation.

In recent years, gel-based polymer electrolytes (PGEs) have emerged as a highly promising alternative, effectively addressing the leakage problem. This research endeavor seeks to harness the potential of gel-based polymer electrolytes to achieve elevated levels of conversion efficiency and enhance the overall energy conversion capabilities of DSSCs.

MSNANO-23 (36)

Tailoring Counter Electrode Performance with Graphene Oxide (GO) and Polyvinylpyrrolidone (PVP) for Enhanced Dye-Sensitized Solar Cells.

Muhammad Shoaib

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Abstract

Graphite served as the initial material for the efficient synthesis of graphene oxide (GO). In the process of synthesizing GO, graphite was sourced from three distinct origins. Notably, employing a four-probe methodology revealed that the highest conductivity was exhibited by GO produced from the graphite electrode of a discharged dry cell battery. The SEM analysis confirmed the layered structure of GO, while XRD analysis verified the creation of graphene oxide by indicating changes in the crystallographic structure resulting from the incorporation of oxygen-containing functional groups. Subsequently, a GO/PVP composite was utilized in the fabrication of the counter electrode for dye-sensitized solar cells (DSSCs). It was observed that the concentration of PVP, functioning as a binder, had a discernible impact on the efficiency of DSSCs. Remarkably, DSSCs featuring a 75% GO counter electrode demonstrated a power conversion efficiency (PCE) of 2.151%, surpassing those employing 70% and 80% GO counter electrodes. Furthermore, this configuration's efficiency exceeded that of conventional platinum-based DSSCs. Collectively, these findings lend support to the potential practicality of employing graphite electrodes from discharged dry cell batteries as a cost-effective alternative to expensive platinum materials in DSSC applications.

MSNANO-23 (37)

Synthesis of silver nanoparticles using green matrix and its application in medical field

Arooj Anwar

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Abstract

Utilization of medicinal plants in medications has tremendous history. Curry leaves (Murraya koenigii) indigenous to our country are known for their vast nutraceutical attributes and can be used for formulation of medicament and food supplements because of their easy availability, no side effects and economical effectiveness. These benefits of medicinal plants have been widely used method to cure a various kind of disease as compared to traditional method. The green biomolecules extracted from curry leaves by decoction and bio binder hydrogel was used to synthesize silver nanoparticles. Extract and hydrogel was analysed by HPLC to identify different bioactives extracted from leaves. The phenolic compounds present in curry leaves extract were Quercetin, Gallic acid, Caffeic acid, Vanillic acid, Chlorogenic acid, M. coumaric acid, Syringic acid whereas xanthan hydrogel displayed the existence of Quercetin, Gallic acid, Caffeic acid, Benzoic acid, p. coumaric acid, Vanillic acid, Chlorogenic acid, M. coumaric acid and sinapic acid. The different functional groups were identified by FTIR in synthesized silver nanoparticles and hydrogel. In both different peaks for stretching frequencies were detected at 3270 (OH, N-H stretching), 2916 (aldehyde and ketone stretching), 2107 (stretching in alkynes), 1438 (C=C stretching in alkenes), 1025 (C-O stretching) and 3263 (stretching of O-H group), 2896 (methylene stretching), 1716 (C=O stretching of carbonyl), 1367 (C-O-C stretching of ether) respectively. The morphological pattern of silver nanoparticles and hydrogel were determined by SEM analysis which shown the spherical shape in AgNPs and elongated shape in hydrogel. Maximum DPPH was shown by silver nanoparticles (52.7±0.67) as compared to aqueous extract and hydrogel (46.9±0.11, 35.6±0.5). The haemolytic activity was found maximum in aqueous extract followed by AgNPs and hydrogel (4.86±0.010, 11.96±2.39, 5.98±0.01) respectively. The maximum biofilm inhibition was shown by hydrogel followed by aqueous extract and AgNPs (51.28546±1.12, 45.49102±1.0236, 42.46811±0.7465) in

staphylococcus aureus whereas in E.coli maximum biofilm inhibition was shown in hydrogel followed by aqueous extract and hydrogel (43.8±0.40, 38.0±0.64, 32.7±1.19). The maximum antibacterial activity of silver nanoparticles, hydrogel and aqueous extract (30.37433±1.47, 22.70667±2.06, 19.86667±1.026) was shown against Staphylococcus aureus as compared to E.coli (27.33333±2.081, 22.70667±2.06, 19.86667±1.026). The maximum efficacy of prepared AgNPs dressing was against staphylococcus aureus (33.16±0.76) followed by E.coli (20.08±2.55) .Thus the results showed that the green synthesized silver nanoparticles had a potential applications in medical field and safe to use.

MSNANO-23 (38)

Silver supported TiO2 Based Nanocomposite for Efficient Round-the-clock Photodegradation of Methylene blue Wasted Water

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Abstract

Dark photocatalysis or Round-the-clock (RTCP) in the recent years has gained attraction for researchers due to serious limitations of conventional photocatalysis. Dark photocatalysis due to its efficiency and economical effectiveness can be employed as robust solution in environmental remediation, wastewater treatment, heavy metals elimination, solar energy harvesting, and hydrogen generation. Nanocomposites of Titanium dioxide TiO₂along with a secondary energy-storing material like silver can effectively be used to drive both light active and dark photocatalysis. The main aim of this research was to develop ceria based composite systems for efficient dark photocatalysis. In practice, Titanium dioxide was prepared using sol-gel route under basic conditions and will be further transform into composites by defined incorporation of any energy harvesting agent like Ag. Prepared systems were characterized by XRD, FT-IR, FT-Raman and SEM/EDX. Photocatalytic efficiency of the prepared systems was assessed against any model dye i.e., and methylene blue (MB) in direct sunlight as well as in darkness. By varying the concentration of energy capturing agent, pH and initial concentration of

M, catalyst loading as well as sunlight and dark exposure times; the photocatalytic performance of Ag-TiO2nanocomposites was optimized for dark photocatalysis. These Prepared systems can be used for water purification applications in near future.

MSNANO-23 (39)

Cu/Co bimetallic oxides for understanding oxygen evolution reaction (OER) of electrochemical water splitting

Anila Tabassum

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Abstract

The depletion of fossil fuels makes the production of hydrogen extremely attractive as an environmentally friendly fuel. However, the process of electrochemical water splitting for hydrogen and oxygen evolution is highly energy challenging. Therefore, construction of a cost effective, bountiful and ecological benign electrocatalyst is thought-provoking. Here, we are reporting straight developed Cu/Co binary oxides on FTO conductive glass slide for the oxygen evolution reaction (OER) of electrochemical water splitting under alkaline medium. The catalysts have been synthesized by simpleminded drop casting method with additional calcination. The morphological survey has revealed fine shaped nanoparticles. The existence of crystalline phase has been determined by X-Ray diffraction (X-Ray). Confirmation of metal oxygen bond has been carried out by Fourier transform infrared spectroscopy (FTIR). The manufactured Cu-Co binary oxides exhibited low onset potential of 130 mV and Tafel slope of 179 mVdec⁻¹ for OER. The durability test conducted for 500 CV cycles depicted their stability and efficacy. Thus, our catalyst showed great potential for OER in electrochemical water electrolysis and crucial for generation of hydrogen fuel.
Keywords: Cu/Co oxides, simple drop casting method, oxygen evolution, water splitting, water splitting, self-standing.

MSNANO-23 (40)

Bismuth doped cerium ferrite: An efficient material as photocatalyst and dielectric material

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Abstract

Bi-doped cerium ferrite Ce_{1-x}Bi_xFeO₃ (x=0.00, 0.01, 0.03, 0.05, 0.07, 0.09) was synthesized via a simple co-precipitation route. The as-synthesized samples were investigated by UV-visible (UV–Vis) spectroscopy, photoluminescence spectroscopy, vibrational Raman and Fourier transform infrared (FTIR) spectroscopies, X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray (EDX) and Brunauer-Emmett-Teller (BET) analyses to study the influence of Bi doping on the optical, structural, morphological and textural characteristics of cerium ferrite. Dielectric studies indicated the charge storage potential of Bi-doped cerium ferrites where a considerable increase in dielectric constant was observed in the case of Ce_{0.93}Bi_{0.07}FeO₃ (1.29178 x 10⁷) compared to the pristine cerium ferrite (1.97615x10⁻¹¹) at 20 Hz. Moreover, small loss tan value of Ce_{0.93}Bi_{0.07}FeO₃ (1.36704) reflected its ability to store charges with minimum current leakage. The prepared samples were also investigated for the photocatalytic degradation of a strong anti-inflammatory drug i.e. diclofenac potassium in aqueous media. The photocatalytic degradation of diclofenac potassium by Ce_{0.93}Bi_{0.07}FeO₃ reached 93% of conversion and was the highest value compared to pristine cerium ferrite (73%), following pseudo-first order kinetics with the rate constant of 0.02038 min⁻¹. This enhanced photocatalytic activity could be attributed to the effective suppression of the charge carriers owed to the crystal defects induced by Bi doping leading to the formation of active species responsible for the degradation of diclofenac. This work established the potential applicability of the ferrite-based composites towards photocatalytic removal of pollutants as well as their use in charge storage devices.

MSNANO-23 (41)

Synthesis and Characterization of CoS/V2O5/rGO-based nano-structured composites material for electrochemical energy storage device

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Abstract

It is crucial to design and manufacture electrochemical energy storage devices that have high power and energy densities along with great cycling ability. Supercapattery demonstrates a hybrid storage mechanism of both a battery and a supercapacitor. The potential use of supercapattery in future electric automobiles, smart power grids, and even in electric and optoelectronic devices which makes it an important electrochemical energy storage device. Supercapatteries are often built with a high-capacity battery-type electrode and a high-rate capacitive electrode. With an appropriate design, it offers certain advantages such as ecological sustainability, superior efficiency, cost-effectiveness, and safety. In the present work, cobalt sulfide and vanadium pentoxide have been prepared by the hydrothermal method, and graphene oxide by modified Hummer method. The prepared composites (CoS/V₂O₅/rGO) were characterized by different techniques and applied as an electrode in supercapacitors and supercapattery. The X-ray diffraction patterns and EDX confirm the successful synthesis of tertiary composites with the average crystallite size of 18 nm. Nanocomposites were grown on the surface of nickel foam. The results demonstrated that valence-rich vanadium material significantly enhanced the redox mechanism. Two-dimensional nanosheets strengthened the three-dimensional geometry, improved the stability and active sites of the structure. The supercapattery device was fabricated by using mixed (AC/Ternary composite) as a working anode and AC as a cathode which was separated by cellulose paper. The evaluation of capacitive and battery mechanisms shows the dominant feature of diffusive and surface-controlled processes at lower and high scan rates respectively due to varying diffusion time of electrolyte species. The fabricated device shows the energy density and power

density of 48.62 Whkg^{− 1}and 1769 Wkg^{− 1} at a current density of 0.5 mAg^{− 1} respectively, with 79 % cyclic stability.

Keywords: Supercapattery, Cobalt Sulfide/ Vanadium pentoxide/Reduced Graphene Oxide,Activated Carbon

MSNANO-23 (42)

Optical and dielectric study of synthesized PVDF-based TiO 2 /ZnO nanocomposites

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Abstract

In this research work, structural, optical and dielectric properties of PVDF based flexible sheets were studied. The X-ray diffraction patterns confirm the development of various phases of PVDF, ZnO, TiO₂ and TiO₂/ZnO. The variation in peak intensities and crystallite sizes are associated with increasing wt.% of ZnO nanofillers. The SEM analysis of polymer-based nanocomposites shows the formation of grain boundaries in the form of colonies which turns into nanoparticles of various dimensions. From the optical properties, the values of energy band gap are found in the range of (4.21-5.25 eV, 3.22-3.15 eV, 3.40 eV) for PVDF, TiO₂ and ZnO respectively. The static value of dielectric constant at 100 Hz is found to be 26.83 for sample D6 (20 wt.%) nanofillers which is 2.05 times greater than pure PVDF and shows relatively low value of loss factor. The maximum AC conductivity of synthesized PVDF/TiO₂/ZnO flexible sheets is found to be 2.06×10⁻⁶ S/m which is 2.63 times larger than PVDF at high frequency (~ 10⁶ Hz) region. The maximum energy density of polymer nanocomposites for wt.% (20%) of ZnO found to be 1.88 J/cm³ at 499 MV/m. Results indicate that a large no. of polymer based nanocomposites chains formed with the addition of wt.% of ZnO/TiO₂ nanofillers which make the NCs more flexible, strengthen and conductive for energy storage applications.

Keywords: Polycrystalline, Band gap, ac conductivity, Dielectric constant, Energy density,

MSNANO-23 (43)

Structural, Electronic, Optical, Mechanical, Thermodynamic and Thermoelectric Properties of ZnSnN2 and ZnMoN2 Ternary Nitrides

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Abstract

The study employs first-principles density functional theory (DFT) calculations employing the generalized gradient approximation (GGA), an extensive exploration is conducted into the structural, electronic, optical, mechanical, thermodynamic, and thermoelectric characteristics of the ternary nitrides ZnSnN₂ and ZnMoN₂. The obtained results demonstrate the mechanical and thermodynamic stability of both nitrides. The computed formation energies for ZnSnN₂ and ZnMoN₂ nitrides are determined to be negative, confirming the structural stability of these compounds. Additionally, the calculated mechanical properties indicate that the studied nitrides exhibit brittle behavior. The results of the elastic anisotropy factors shed light on the anisotropic behavior of ZnSnN₂ and ZnMoN₂ nitrides. Both nitrides exhibit low reflectivity in the infrared and high reflectivity in the ultraviolet regions of the electromagnetic spectrum. In the visible region, an average reflectivity of approximately 20–35% is observed, indicating that these nitrides possess the potential to enhance light absorption in solar panels and can be applied for anti-reflective coatings in optical devices. The study also encompasses the calculation of thermodynamic properties under various pressures, with corresponding discussions on the results. Furthermore, the investigation into the Debye temperature to explore the vibrational response of the studied nitrides. Thermoelectric properties are assessed using the Boltztrap2 code. Collectively, the analyses of mechanical, optical, thermodynamic, and thermoelectric properties indicate that these nitrides have the potential to be well-suited for electronic, optical, and energy storage devices. Additionally, their notably high ZT values underscore their potential as outstanding thermoelectric materials.

MSNANO-23 (44)

Laser-induced breakdown spectroscopy coupled with machine learning for identification of ionization states of oxide materials

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Abstract

Laser induced breakdown spectroscopy (LIBS) is a well-known type of atomic emission spectroscopy, which is being used to identify the elements present in any sample. In current study, LIBS technique was used to detect environmental parameters and analyze the ionization states of iron oxide such as Fe₂O₃ and Fe₃O₄. In this technique, Nd-YAG laser was used to identify ionization states. Iron oxides were being studied and analyzed including elemental characterization, determination of plasma temperature and electron number density, peak identification, LTE conditions in the 200–600 nm range of LIBS spectrum. A clear variance in the samples was seen which provides a quick and efficient way to separate sample classes with little elemental changes. Supervised and unsupervised models of machine learning techniques were used to get better results for identification and classification purposes. Electrical conductivity of prepared samples was also determined.

MSNANO-23 (45)

g-C3N4/graphene oxide/SnFe2O4 ternary composite for the effective sunlight-driven photocatalytic degradation of methylene blue

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Abstract

A broadly used dye, methylene blue (MB), adversely impacts human health and water resources, which triggers efficient methods for its elimination. Semiconductor-based heterogeneous photocatalysis is an environmentally friendly approach that effectively degrades organic pollutants. The purpose of the present study is to elucidate and validate the application of a promising g-C₃N₄/GO/SnFe₂O₄ (CGS) composite for the degradation of methylene blue dye. The ternary CGS composite has been synthesized using an in situ solvothermal approach. The synthesized composites were analyzed through FTIR, XRD, SEM/EDX, TEM, XPS, and UV–VIS spectroscopy. The photoactivity of composites and affecting parameters (pH, H₂O₂ dosage, composite amount, initial dye concentration, irradiation time) were observed in sunlight illumination. The optimal conditions for photocatalytic degradation were pH = 5, photocatalyst dosage = 30 mg/100 mL, H₂O₂ dosage=6 mM, and initial dye concentration (IDC) of 10 ppm using ternary CGS composite and MB dye was degraded effectively within 1 hr. 98% degradation efficacy was attained by using ternary CGS composite under the optimized conditions. Scavenging analysis suggested that [•]OH radicals were the key reactive oxygen species (ROS) responsible for the photodegradation of MB dye. Furthermore, the CGS nanocomposite exhibited outstanding recyclability of 84% after five consecutive runs, demonstrating its potential for use in practical applications, particularly pollutant removal.

MSNANO-23 (46)

Analysis of whole blood samples using Laser Induced Breakdown Spectroscopy coupled with machine learning

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Abstract

Laser-induced breakdown spectroscopy (LIBS) is an advanced kind of atomic emission spectroscopy (AES). LIBS is a future superstar, which is being used to identify the elements present in the sample. This technique allowed a laser beam to be focused on the sample surface which atomizes the sample of whole blood samples such as breast and ovarian cancer. All ionized elements present in plasma produce light corresponding to certain and unique atomic energy levels and that plasma light was transmitted to the spectrometer via optical fibers. LIBS was used to analyze including elemental characterization, determination of plasma temperature, electron number density, peak identification, and LTE conditions in the 190-600 nm range of LIBS spectrum. Principal component analysis (PCA) was an unsupervised machine learning model and other supervised models of machine learning were applied to get better precision and identification purposes. A biological sample of the blood of healthy and diseased patients was studied and analyzed using LIBS. The spectral lines were analyzed by the NIST database then the PCA model and other machine-learning methods were applied. The LIBS technique, combined with the chemometrics method, was used to detect and discriminate against human malignancies in a fast less invasive, and accurate manner.

MSNANO-23 (47)

Enhanced photo-catalytic degradation of reactive dyes under UV/Visible light irradiation using efficient metal oxide nanocomposites

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Abstract

The world is worried about the harmful impacts of textiles on the ecosystem. It is therefore necessary to degrade these dyes from water by appropriate methods. Metal oxide Nano-composites have shown great promise in the domain of water cleanup in last few years. Photocatalysis techniques are used to develop methods for removal or decomposing contaminants from aqueous solutions. For this purpose Rare Earth Metal Dy dysprosium doped ZnFe2O4 [Fe1.0936DyZn0.8064] were prepared with different concentrations such as (x= 0.02, 0.04, 0.06, 0.08, 0.10) by using a technique co-precipitation. The functional, structural, optical, magnetic, and properties of degradation of this dysprosium doped particles were analyzed using different characterizations like size of crystallite (D) and various parameters (oxygen positional parameters, distribution of cation and bond length) were found out by utilizing XRD (X-ray diffraction) and it was noted that as the concentration of dy3+ ion enhanced the size of peck decreased and the size of grain kept within nano regime, which intern impact on the surface area. Different functional parameters such as interionic bonds, elastic, and ion distribution were found using FTIR. SEM was used to investigate the size of the sample. UV-Vis spectroscopy was used to analyze the optical properties of the prepared metal oxide nanocomposites. Under sunlight as-synthesized dysprosium doped ZnFe2O4 at concentration x = 0.10 showed a degradation activity against RhB (Rhodamine B), its degradation efficiency was noted to be 86% after 90 minutes at different optimized conditions such as range of pH=8, catalyst dose=30mg/100 ml, oxidant dose=10mM, time of irradiation=120 minutes and concentration of Rh B= 50 ppm.

MSNANO-23 (48)

Elemental Analysis of Doped Metallic Nanoparticles by Using Laser Induced Breakdown Spectroscopy

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Abstract

Laser-induced breakdown-spectroscopy (LIBS) is a short pulsed laser which is centered on specimen to create plasma of high temperature. Due to quick sensitive optical-diagnostic, LIBS is currently being used to detect the specific species. In this experiment, a Q switched Nd-YAG laser of particular energy and specific wavelength used in order to record the spectra created by laser induced breakdown spectroscopy (LIBS) of sample. Numerous techniques have been described in the most recent decade, multi-beat LIBS, reverberation LIBS and different hyphenated procedures. Elemental analysis of nanoparticles directly analyzed by using Laser induced breakdown spectroscopy. The sample of different particle size take. By the aid of LIBS, plasma created on different samples of nanoparticles. The recorded elemental data of samples compared with National Institute of Standard and Technology. All the elements present in the synthesized NP sample will be determined plasma temperature and electron number density calculated and local thermodynamics equilibrium condition verified. Calibration-free LIBS (CF-LIBS) was used to quantitatively analyze the concentration of elements in a sample in local thermodynamic equilibrium conditions.

MSNANO-23 (49)

Optimizations of Zr/rGO/CeO2-Based Nanocomposites for Optoelectronics Applications

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Abstract

Perovskite solar cells, light-emitting diodes, and lithium-ion batteries have been considered emerging optoelectronic devices. Solar cell and perovskite solar cell efficiency has increased by using optimal nanocomposites. The major techniques (sol-gel method) have been premised on inorganic materials to optimize many perovskite solar cells in experiments. Perovskite solar cells (PSCs) have greater spectral purity, a longer lifetime, and lower energy consumption. The perovskite halide-based absorbing material separates the energy transfer layer (ETL) and the hole transfer layer (HTL). These two layers are critical for maintaining air consistency and raising power conversion efficiency (PCE). In this research, Zirconium nanoparticles have been optimized by the sol-gel method. Reduced Graphene oxide nanoparticles have been optimized by hummer methods with H₂SO₄, KMnO_{4,}H₂O₂, and HCl with different concentrations. Cerium oxide nanoparticle has been optimized by using the sol-gel method. The solution of nanomaterials has different concentrations of H₂SO₄, KMnO_{4,}H₂O₂, NaOH, and NaNO₃. Sol-gel methods have been used to optimize the Zr/rGO/CeO₂nanocomposites. SEM, XRD, Raman, CV, and UV-visible light have been used to examine the surface morphology, crystallinity, and absorbance to characterize optimized nanocomposites.

Keywords: Zirconium/ Reduced Graphene Oxide, Cerium Oxide, Optoelectronics Devices

MSNANO-23 (50)

Analysis of blood serum using Laser Induced Breakdown Spectroscopy coupled with machine learning

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Abstract

Laser induced breakdown spectroscopy (LIBS) is a well-known type of atomic emission spectroscopy, which is being used to identify the elements present in any sample. In current study, LIBS technique was allowed a laser beam to be focused on the sample surface which atomizes the sample of whole blood serum samples such as breast and ovarian cancer. All ionized elements present in plasma produce light corresponding to certain and unique atomic energy levels and that plasma light was transmitted to the spectrometer via optical fibers. LIBS was used to analyze including elemental characterization, determination of plasma temperature, electron number density, peak identification, and LTE conditions in the 190-600 nm range of LIBS spectrum. Principal component analysis (PCA) was an unsupervised machine learning model and other supervised models of machine learning were applied to get better precision and identification purposes. Cancer and non-cancer samples were the same elemental composition. Few emission lines can be detected in less amount. I detected fully distinguished the blood and serum. The malignancies were diagnosed using serum samples that dip on the substrate. The LIBS technique, combined with chemometrics methods, was used to detect and discriminate human malignancies in a fast less invasive and accurate manner. A biological sample of serum of healthy and diseased patients was studied and analyzed using LIBS with machine learning.

MSNANO-23 (51)

Hydrothermal synthesis, characterization and photocatalytic performance of Carbon quantum dot supported CeO2 photocatalysts.

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Abstract

Industrial wastewater and textile pollutants water is a severe threat for living organisms on earth. Processes for the active removal of contaminants from wastewater are therefore continuously improved to address this issue. One of the promising potential approaches is sun-driven photocatalysis using low-cost metal oxides to purify dye-contaminated wastewaters. This research aims to prepare ceria-based nanocomposites for efficient sun-driven water purification of organic and biologically affected wastewaters. In practice, CeO2 NPs were synthesized by sol-gel method. Cerium nitrate hexahydrate was used as a basic precursor to synthesize ceria nanosol. Subsequently, CQDs were doped to CeO2 as support to form CQDs-CeO2 nanocomposites. The CeO2 CQDs were synthesized by controlled mixing with carbon quantum dots (CQDs) into nanosol via sonication at pH=8 and were subjected to hydrothermal route at defined treatment conditions. Prepared nanomaterials were characterized by XRD, FTIR, as well as SEM/EDX. The photocatalytic performance of the prepared nanocomposite was tested against model and industrial wastewaters in direct sunlight. Performance was further optimized by varying CQDs-CeO2 concentration, the initial concentration of contamination, pH of eluents as well as catalyst loading and exposure timings.

MSNANO-23 (52)

Insight into Methylene Blue removal using ZnO/Co3O4 Photocatalyst

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Abstract

The release of dye pollutants into reservoirs is harmful to aquatic life and poses serious health risks to humans, which is a significant issue everywhere in the world. Photocatalytic degradation of organic dyes has attracted the attention of researchers in order to purify industrial wastewater. In this work, ZnO is incorporated with Co₃O₄ using the template-free hydrothermal method and homogeneous co-precipitation method. After studying the structural and morphological characteristics with XRD and FESEM, optical properties and bandgap was investigated using UV Visible spectra, which gives information about the alterations in the band gap of nanocomposite while revealing defects in the materials. The photocatalytic activity was investigated for methylene blue (MB) over the tenure of 60 minutes. The composite exhibited 3.1- and 5.3-times better degradation as compared to pristine Co₃O₄ and ZnO, respectively.

MSNANO-23 (53)

Enhancing Methylene Blue Photodegradation with Silver-Doped ZnO Nanoparticles

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Abstract

This study presents a simple and efficient hydrothermal method for synthesizing silver-doped zinc oxide nanoparticles. The synthesized nanoparticles were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), UV-visible spectroscopy, Fourier-transform infrared spectroscopy (FTIR), and photoluminescence (PL) spectroscopy. The results confirmed the successful doping of silver into the zinc oxide lattice and the formation of nanoparticles with a hexagonal wurtzite structure.The photocatalytic activity of the silver-doped

zinc oxide nanoparticles was evaluated for the degradation of methylene blue under ultraviolet (UV) light irradiation. The nanoparticles exhibited remarkable photocatalytic activity, degrading methylene blue completely within 60 minutes. The high photocatalytic activity can be attributed to the synergistic effect of silver doping and the large surface area of the nanoparticles. Cyclic stability studies were conducted to assess the long-term applicability of the photocatalyst. The results showed that the nanoparticles retained their photocatalytic activity even after five cycles of use. The influence of solution pH on photocatalytic activity was also investigated. The results revealed that the photocatalytic activity was highest at neutral pH. Scavenger experiments were conducted to identify the active species involved in the photocatalytic process. Overall, the results of this study demonstrate that silver-doped zinc oxide nanoparticles are a promising photocatalyst for wastewater treatment and environmental remediation applications.

MSNANO-23 (54)

Bandgap Tunning of Zinc Oxide Heterostructure for Improved Photocatalytic Performance under Solar Irradiation.

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Abstract

Herein, we report the fabrication of Zinc Oxide (ZnO)/g-C3N4 nanocomposites using a hydrothermal process. Different physiochemical properties of the as-fabricated material were tested with the help of XRD, SEM, EDX, FTIR, UV-Visible and PL spectroscopy. XRD analysis confirmed the fabrication of the material and crystalline size was calculated. SEM micrographs exhibited the unique surface morphology. EDX provided the elemental analysis. FTIR spectroscopy tracked the sample purity. The bandgap measurements were performed using Tauc plot with the help UV-Visible spectroscopy, that are consistent with PL spectroscopic analysis. The photocatalysis response of ZnO/g-C3N4 was tested by the decomposition of organic dye under visible light illumination for a time of 80 minutes. The large surface area of the particles favours the improved photocatalytic ability of the fabricated particles. This work proves useful for fast and the economical fabrication of ZnO/g-C3N4 nanocomposites for the photocatalytic degradation of water pollutants.

MSNANO-23 (55)

Effect of external fields on synthesis of laser ablated gold nanoparticles and study of their photothermal response

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Abstract

Nanotechnology has diverse applications in the field of science. Nanoparticles are such particles which have size range in nanometer. Laser ablation is a promising technique used to synthesize the NPs of different materials having different size and shape. It is simple, fast and environment friendly method to prepare the NPs in one or two steps without using any external chemical agent. In this work, gold nanoparticles was used which have numerous applications in different fields like in medical for cancer treatments, in biology for optical imaging, in cosmetics and for environment to make sensors. Nd YAG laser having wavelength of 1064 nm, pulse duration 6 nsec, repetition rate 10 Hz and pulse energy of 290 mJ was used to synthesize the AuNPs. A convex lens with a 10 cm focal length was employed to focus the laser beam on the sample. The sample was immersed in 10 ml distilled water and total ablation time was 3 minutes. In this work, it was investigated that, how temperature affected the production of gold nanoparticles. We also investigated the effect of external electric and magnetic field. These external fields significantly enhanced the size and concentration of gold nanoparticles. By varying the temperature and electric field, we were able to identify the considerable variations in the size and concentration of gold nanoparticles. After synthesis, UV-Visible spectrophotometer was used to check the absorption properties of our samples. We also calculated the band gap of AuNPs by using Tauc plot method. Furthermore we have checked the photothermal response of these synthesized gold nanoparticles in phantom with diode laser. The result showed that AuNPs shows good biocompatibility and can be used in biophysical application.

MSNANO-23 (56)

Optical, Structural, and Morphological Properties of Ag-doped CuO Nanoparticles

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Abstract

Metal and metal oxide nanoparticles have novel applications in optical, electrical, mechanical, and optoelectronic devices. Silver (Ag), which belongs to the noble family of metals, has gained a lot of interest in the scientific community due to its high electrical and thermal conductivity. Due to their unique features and potential uses, copper oxide (CuO) nanoparticles (NPs) have attracted a lot of attention as compared to the other metal oxides that are commonly used in a variety of applications including catalysts, sensing, water treatment, and electrical devices. CuO NPs exhibit maximum absorbance in the UV range, due to high absorbance, exceptional and optical properties, CuO is one of the potential candidates in the photovoltaic industry. In this research work, we were interested in seeing the effects of doping of Ag on the optical, structural, and morphological properties of CuO NPs. In order to achieve this objective, first CuO nanomaterial was synthesized by using the co-precipitation method. Later, Ag was doped in the locally prepared CuO nanostructures to check the different properties of Ag-doped CuO NPs. The structural, morphological, and optical properties of the doped and undoped CuO were studied by using state-of-the-art techniques, like X-ray diffraction (XRD) in which two prominent 2Ɵ peaks observed at 35.35 and 38.55° correspond to (002) and (202) representing CuO NPs exhibited an average crystal size of 7.28nm, one prominent 2Ɵ peak and the three less intense peaks observed at 37.98, 44.05, 64.22, and 76.79° corresponds to (111), (200), (202), (311) represent the Ag doping into CuO NPs with the average crystalline size 11.19nm, result an increase in crystallite size by doping. Scanning electron microscopy (SEM) analysis was carried out to study the morphology of pure and Ag-doped CuO NPs prepared via the coprecipitation method which was spherical in shape. UV-visible spectrophotometers have bandgap values of 2.25eV for pure and 1.9eV for Ag-doped CuO. FTIR spectra sharp absorption bands between 400 and 900 cm⁻¹of CuO NPs, and doped NPs exhibited two sharp absorption peaks at 570 cm^{–1} and 835 cm^{–1}, and Ag doped CuO exhibits peaks at 795 and 881 cm^{–1}.

Keywords: Optoelectronic, Nanoparticles, Copper oxide, Morphology

MSNANO-23 (57)

Synthesis and characterization of NiCo2O4 based nanocomposites for energy storage applications

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Abstract

Metal oxide based nanocomposites have been considered as promising electrode material for lithium ion batteries with improved reversible capacity, structural stability and cyclic stability as compared to single metal oxides. NiCo₂O₄ nanocomposites with rGO in controlled morphology, shape and size were synthesized by using hydrothermal method. The nanorods were prepared in pure NiCo₂O₄. Mesoporous sheets like structures with average diameter of 12.2 nm and length of about 5µm were synthesized. The synthesized material was characterized by scanning electron microscopy (SEM), X-ray diffraction analysis (XRD), Fourier transform infrared spectroscopy (FTIR) and energy dispersive X-ray spectroscopy (EDX). The coin cells were fabricated in the inert environment by using Argon Glove Box. Numerous electrochemical tests, including cyclic voltammetry (CV) and galvanostatic charge discharge (GCD) were successfully performed by using battery testing system to investigate the stability and efficiency of synthesized composite as the battery electrode. The first discharge capacity at current density of 50 mAg⁻¹ was 1410 mAhg⁻¹with the columbic efficiency of 98 %. After 100 cycles it retained the capacity of 98 % at current density of 300 mAg⁻¹ which showed its high cyclic stability, good cyclic performance and long cycle life.

MSNANO-23 (58)

Synthesis and Characterization of Zr/CeO2-Based Nanocomposites for Optoelectronic Devices

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Abstract

The progress of optoelectronic devices started in the early 1960s with the development of the LED and presently thereafter the laser and solar cells. In perovskite solar cells, light emitting diodes, and laser diodes, light absorption, and power conversion efficiency could be optimized. Perovskite solar cells have been considered the main application of the optoelectronic device. The major problem of perovskite solar cells is low efficiency with instability. The sol-gel method has been used to synthesize Zr nanoparticles and the hydrothermal method has been used to synthesize CeO₂ nanoparticles to successfully create the Zr/CeO₂ nanocomposites. This standard has been due to increased requirements for good performance and advanced determination among consumers. To characterize the Zr/CeO₂ nanocomposites, SEM, X-ray diffraction (XRD), and UV/Vis have been used for surface morphology, crystal morphology, and absorbance. The size and shape of the samples have been determined using scanning and transmission electron microscopy (SEM and TEM). Transmission electron microscopy (TEM) has been used to estimate the size of the Zr nanoparticles. Finally, Zr/CeO₂ nanocomposites have been used to enhance the efficiency of optoelectronic devices

Keywords: Zirconium, Cerium Oxide, Nanocomposites

MSNANO-23 (59)

Polar wood modification by ethylene Glycol dispersion

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Abstract

Wood is very promising building material with numerous benefits but has equally drawbacks and short-comings as well such as shrinkage, swelling, biodegradation, and low fire-resistance. Wood contains cellulose and hemicellulose which have OH groups that make wood hydrophilic. To overcome the hydrophilicity, OH groups must be blocked or attached by any chemical that leads to hydrophobic wood with improved decay and weather resistance. In this research, ethylene glycol dispersions and impressions are assessed for their potential in improving water-related properties and fire retardancy characteristics in wood. In practice, Water solutions of ethylene glycol of defined concentrations and compositions will be vacuum impregnated into the poplar sapwood and treated wood was dried in air and finally cured to get modified-end products for basic characterization employing FTIR, SEM and tested. Treated wood surface morphology characterized by SEM and distribution of ethylene glycol within wood analyzed by EDX. Further, any chemical attachment established between wood and impregnating material studied by FTIR. Finally testing physical properties such as water linked property (leaching resistance, degree of hydrophobicity, relative water and moisture sorption, equilibrium moisture content (EMC) and ASE etc.), of treated wood in relation to untreated sample was lowered. A significant improvement in dimensional stability was seen in EG treated wood with regards to anti-swelling efficiency (ASE), and comparison of modified wood's fire retardancy to untreated wood has been conducted, and due to its low cost and ease of handling, this treatment has vast potential for commercialization.

MSNANO-23 (60)

Synthesis and Characterization of Ga2O3 Thin Films Deposited on Si(110)

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Abstract

The approach of nanotechnology turns every field of life through its accomplished applications in different fields. The administration of this technology turns dark lives into a glow. The requirements of nanotechnology increased day by day. Ga₂O₃ is a novel semiconductor having wide-bandgap and its thin films are being used in power electronics, optoelectronics, and sensors. Keeping in view the importance of this material, proposal was prepared to synthesize Ga₂O₃ thin films onto single crystal substrates. In order to achieve this objective, first of all Ga₂O₃ nanomaterial was prepared. The substrates were cleaned through ultrasonic cleaning and acetone to remove the biological contaminations. Later on, thin films of Ga₂O₃ were prepared onto the substrates by using a very simple spin coating technique. The prepared thin films were characterized for the structural, optical, and morphological properties by using well known tools like X-ray diffraction, UV-Visible spectrophotometer, scanning electron microscopy (SEM), respectively. These techniques provided information about the Ga₂O₃ thin film where XRD pattern appear and the intensity of the substrate peak was increased for grown films, UV exhibits the absorption spectra in the UV and visible range. SEM confirms the amorphous nature of crystal visible in figure and the fine microstructure and uniform distribution of dense particles of Ga₂O₃ films grown. XRD patterns have two prominent 2θ peaks observed at 34° and 69.71° correspond to the (0 2 0) and (2 0 0) peaks of silicon (Si) at temperature of 400°C. A intense absorption peak for Ga2O3 films at 350nm is mentioned with red color observed at 500 °C with the bandgap 3.54eV, and the peak at 300nm mentioned with black color observed at high temperature 800 °C with bandgap value 4.1eV. The SEM analysis shows that the by increasing the temperature from 400 to 800 °C surface show grain boundary.

MSNANO-23 (61)

Investigation of Cr3 Doped CuGao2 as an inorganic Hole Transport Material (HTM) forPerovskiteCells

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Abstract

Perovskite Solar Cells (PSCs) are becoming a feasible method for developing effective energy harvesting devices. The biggest obstacles to their commercialization are their high price and lack of ecologically stable organic hole transporting materials (HTMs). CuGaO₂ provides high coordination, stability, and low-temperature processing for effective and reliable PSCs. Here, a variety of solid solutions of CuGaO₂ and CuCrO₂ were created by a hydrothermal process to obtain the ideal composition that results in reliable size control and high hole conductivity employed for surface passivation at the perovskite contact. The composition range of CuGaO₂doped with Cr⁺³ were CuGa_{1-x}Cr_xO₂ ($0 \leq x \leq 1$, CuGaO₂). XRD patterns were obtained for the particles of various compositions, these (006), (012), (104) and (024) having 2 values 33.23°, 36.48°, 43.43°, and 50.43° peaks were identified without the appearance of any impurity peaks. The optical properties of nanoparticles were studied using UV-visible spectroscopy that showing the bandgap of CuGaO₂ was decrease from 3.32 eV to 3.05 eV. The chemical properties of nanoparticles were studied by using Fourier transform infrared spectroscopy that indicates the presence of metal oxide groups of bending and stretching vibrations. J-V curves of perovskite solar cell devices were applied, the altered system achieve a PCE of 16.9%, when the concentration of Cr³⁺ was added in CuGaO₂ is 30%. This research opened up a fresh path for the logical design of extremely stable and effective Pscs.

MSNANO-23 (62)

ynthesis, Preparation and Properties of 2D-Graphene for Electrochemical Energy Storage and Conversion

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Abstract

Stimulating properties of Graphene, like its vast surface area, exceptional electrical conductivity, extreme thinness, amazing electron kinesis, and state-of-the-art mechanical regulation, have added an enormous investigative concern. These topographies are mostly vivacious for numerous electrochemical energy storage devices (EESDs), e.g., Li-Sulphur batteries, Lithium Ion batteries, Lithium Oxygen batteries, Sodium Ion batteries, super capacitors, hybrid cathode, and anode materials. Scaled-up, stable production and correspondence of carbon-based nano materials is an essential condition for developing Graphene-based EESDs. This chapter diagnostically includes the preparation methods of Graphene and properties of Graphene nano materials with various dimensions in adaptable EESDs. The main challenges and prospects in this field are also discussed.

MSNANO-23 (63)

GREEN SYNTHESIS OF AgO NANOPARTICLES WITH AZADIRACHTA INDICA AND TURMERIC ROOTS FOR ANTIMICROBIAL APPLICATIONS

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Abstract

Nanoparticles typically have high responsiveness and massive surface-to-volume ratio that increases their probable antimicrobial applications. In current research work, green fusion of Ag nanoparticles was accepted by using Azadirachta Indica to attain desired morphology of final product. In biosynthetic procedure Azadirachta Indica was used along with main precursor of Ag nanoparticles. In next step available characterization e.g., XRD, SEM, UV-Visible spectroscopy and FTIR was performed for confirmation of structural, morphological, optical analysis and functional group presence. In addition, comparison of synthesized Ag nanoparticles size, shape and relevant properties was investigated while using room and annealed temperature. Finally antimicrobial activity of final product was assessed by using culturing procedure. XRD analysis depicted the Face Centered Cubic structure of green synthesis of Ag nanoparticles. SEM

analyzed the morphology of nanoparticles at the several magnifications like x7442, x1948, and 3472. FTIR showed that the compounds of bimolecules are accountable for reduction of Ag+ ions to Nps of Silver. So, these findings had exposed viewpoints for upcoming inquiries concerning the usage of these silver nanoparticles as antimicrobials in the ranges of health cares.

MSNANO-23 (64)

Hydrothermal synthesis and characterization of CoCrAl Heusler alloys

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Abstract

Heusler alloys have sparked the interest of scientists due to their possible application in spintronic devices. These alloys are named after Fritz Heusler, a 19th-century German mining engineer and chemist. The most important property of Heusler alloy is half metallicity. Spin-up electrons cross the fermi level and show conducting or metallic behavior. While spin down electrons does not cross the fermi level and give a band gap. Because of this half-metallicity property, they show 100% spin polarization. Spintronic is an emerging field in nanoscale electronics that uses the spin of electronics, rather than an electric charge to encode and process data. Half metallic materials with complete spin polarization at the fermi level are highly attractive for spintronics applications because of their high spin polarization. Spintronics is the new emerging field that recasts modern information technology using electron spin along with its charge. Various spintronic devices have been under research for the last few years such as GMR-based devices, MRAMs, etc. These devices are based on conventional ferromagnetic material that exhibits spin asymmetry. Half-metallic ferromagnetic materials, especially Heusler alloys, are considered as most promising candidates because of high spin polarization

MSNANO-23 (65)

Photocatalytic degradation of Direct Red 28 by Polyorthoanisidine/g-C3N4/TiO2 ternary composite

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Abstract

Industrial dye effluents cause serious environmental concern. The methods for the treatment of dyes include biodegradation, coagulation, adsorption, advanced oxidation process (AOP), photocatalysis, and the membrane process. In this study, graphitic carbon nitride, TiO₂(nanoparticle) and poly-o-anisidine was used to synthesize ternary composite Polyorthoanisidine/g-C₃N₄/TiO₂ a photocatalyst. The characterization of synthesized composite material was carried out using different techniques such as Fourier transform infrared (FTIR) scanning electron microscopy (SEM), X-ray diffraction (XRD), and UV-visible spectroscopy. This composite, a photocatalyst, follows advanced oxidation process and employed for degradation of toxic dyes into nontoxic product. This photocatalytic activity was investigated by employing composite in aqueous solution of Direct Red 28 under UV-Vis irradiation. This composite degrades Direct Red 28 dye at 20mg/L at pH 4, 7 and 240min almost 100%. Used composite showed 87% degradation of Direct Red 28 after four consecutive cycles indicate that Polyorthoanisidine/g-C-₃N₄/TiO₂nanocomposite is a stable and efficient catalyst. The high reusability and efficiency of the Polyorthoanisidine/g-C-₃N₄/TiO₂ nanocomposite is due to enhanced visible light absorption effect of the g-C₃N₄ and polyorthoanisidine.

MSNANO-23 (66)

From Lab to Ocean: A Visionary Approach to Oil Spill Cleanup Using Dual-Function Polymeric Nanomaterials

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Abstract

The implementation of photocatalytic approaches to treat petroleum waste (diesel) in the ocean has gained popularity recently, although there are now just a few photocatalytic technologies available for petroleum degradation. The treatment of marine oil spill pollution with dispersant proved to be effective enough but traditional dispersants only exhibited monolayer oil dispersion. This study suggested utilizing modified metal semiconductors with aminophenol formaldehyde (APF), a very effective particle dispersion with photocatalytic activity, to remove oil pollution from the ocean. We fabricated effective photocatalytic nanocomposites using a simple solvothermal synthesis process to dregs the metal semiconductors TiO2 and Fe3O4 in the conducting APF polymer (MAPF and TAPF). These materials could drift on the water's surface with high adsorption capacity and diesel degradation. TiO2-APF (TAPF) revealed both exceptional oil spill scattering and assisted photodegradation simultaneously. The diesel oil droplets isolated by TAPF exhibited greater stability, which is directed towards symbiotic emulsification reciprocation between TiO2 and APF in sea water. According to the findings from the experiments, MAPF and TAPF both exhibit good photocatalytic performance, with up to 74% and 86%, respectively. As a result, the suggested combination of dispersion, adsorption and photocatalysis will offer a revolutionary strategy to significantly facilitate the management oil spills on sea water.

MSNANO-23 (67)

Cost effective Co-precipitation method for synthesis of iron oxide nano-crystallites for bioremediation of organics and heavy metals from wastewater

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Abstract

Iron oxide nanoparticles can help in wastewater treatment in a more organic, well-organized and less costly way. The synthesis and characterization of iron oxide nanoparticles, specifically Fe_2O_3/Fe_3O_4, for wastewater improvement was done. They have some properties including high reactivity, significant surface area, functionalization capabilities, oxidizing properties and adsorption of contaminants. We have analyzed the function of iron oxide nanoparticles in cleaning up dirty water by checking their size and crystal shape. The weighed amount of $FeCl_2.4H_2O$ (3g) was added into the flask, which was continuously and steadily stirred. Then standardized 100 ml ammonium hydroxide solution was loaded with 0.7 mole ammonium hydroxide and then ammonia solution was added with the rate 0.007 mole/sec followed by stirring for one second. The total volume of the mixture was 200ml in the end of the process. After the system reached a precipitation state, it was allowed for cooling and settling of the precipitate in the bottom of the flask. The precipitate was dried at 100 ℃ for 1 hour in a vacuum. We used characterization techniques like X-ray diffraction (XRD) to show that the magnetic nanoparticles were pure Fe_3O_4 with a spinel structure. The nanoparticles were characterized by XRD, Scanning Electron Microscopy (SEM), and Transmission electron microscope (TEM). The cell thickness of nanoparticle approximated in the range of 5.65- 8.16 nm whereas the particle size in the TEM was 20-22 nm. In this research attempts were made to study their effectiveness and the findings were proved by opting biological method (bio-film) which was found to be very effective bio-remediation method with the removal of 91% organics and heavy metals from waste water.

Keywords: XRD, SEM, TEM, bio-remediation method

MSNANO-23 (68)

Sol gel Synthesis of Zinc oxide nanoparticles, its characterization and application as economical sunscreen

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Abstract

Zinc oxide plays an important role due to its special characteristics such as anti-corrosion, anti-bacterial, has low electrons conductivity and excellent heat resistance. Therefore, in this studies zinc oxide nanostructures were synthesized by using sol-gel method . Sol-gel method is the simplest method and has the ability to control the particle size and morphology through systematic monitoring of reaction parameters. Gel-based ZnO nanoparticles were synthesized via sol gel method using Zinc acetate dehydrate ($Zn(CH_3COO)_2.2H_2O$) as a precursor and ethanol (CH_2COOH) was used as solvent, Sodium hydroxide (NaOH) and distilled water were used as medium. Gel-based ZnO NPs were characterized by using SEM, XRD, EDX and FTIR. Furthermore, their effectivity as sunscreen was analyzed by studying their biological properties on various bio-films.

Keywords: Gel-based ZnO nps, XRD, EDX, SEM, biological properties, bio-films

MSNANO-23 (69)

Optical and Thermoelectric Properties of Aluminum Doped Cobalt Sulfide

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Abstract

Metal Chalcogenides focus on the cobalt sulfides' nanoparticles due to its emerging optical, electrical, size dependent, electrochemical and catalytic properties. It's one of the utmost sophisticated metal sulphide complexes with different phases and contrast chemical compositions, along with Co_9S_8, Co_3S_4, CoS, CoS_2, Co_4S_3, Co_2S_3 and $Co_{1-x}S$. In this work, pure configuration of cobalt sulphide and Aluminum (Al) doped cobalt sulphide with the number of complexations was examined using co-precipitation method. As S-source we used Sodium Sulphide (Na_2S) and as a precursor Aluminum Chloride and Cobalt Chloride ($CoCl_2$) was used. We used different concentrations of Aluminum (Al) on Cobalt Sulphide Nanoparticles, for the analysis of different properties like optical properties and structural properties. The X-ray Diffraction (XRD), Scanning-Electron-Microscopy (SEM), Fourier-Transform-Infrared-spectroscopy (FTIR) and Energy-Dispersive X-ray (EDX) was done for the investigation of the structure, crystalline size, shape and optical properties of the pure Cobalt-sulphide (Co_9S_8) and the Aluminum-doped samples ($Co_9Al_{0.10}S_8$, $Co_9Al_{0.15}S_8$, $Co_9Al_{0.20}S_8$, $Co_9Al_{0.25}S_8$). The structural shape, Lattice parameters and other microstructural properties was investigated through the X-ray-Diffraction (XRD). In further study it came to know that the crystalline size varies with the change in the concentration of the Aluminum material in the samples. The least crystalline size that calculated was 20 nm. SEM analysis used for the study of the morphological behavior and properties of the all-synthesized samples. SEM helps to calculate the grain size of the particles within the prepared samples. The average grain size that was observed from the Scanning-Electron-microscopy (SEM) is lie between the 50nm to 70nm. Energy-Dispersive X-ray showed the presence of the organic elements that was remained unburnt. FTIR absorption band is between 250 cm^{-1} to 750 cm^{-1}.

Keywords: Co-precipitation method, XRD, EDX, SEM, FTIR

MSNANO-23 (70)

Up-gradation of Bioavailability Plants of cheng-kruk and apple of Sodom by using Nano Suspension Technique as a water-soluble antimicrobial nanomedicine

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Abstract

An important aspect for drug efficiency is solubility. For developing new pharmaceutical products solubility is major challenge. The resistance of weakly water-soluble medications to be dissolved into the liquid is a limiting factor for their performance. Optimizing bioavailability requires escalating the dissolution rate of weakly water-soluble medicines. Nanosuspensions are colloidal dispersions of drug particles in a liquid segment that are sub-micron in size. The Nanosuspensions can be utilized to reframed accessible medications to eliminate toxic undesirable compound. it was intended to shape nanosuspensions by utilizing natural medications, to upgrade their disintegration rate and bioavailability. Sono-precipitation procedure was utilized to get ready nanosuspensions by utilizing SDS (Sodium Dodecyl Sulfate) as a stabilizer. Drug powder was disintegrated in natural dissolvable independently. Then, at that point, it was blended in with stabilizer arrangement. The blend was homogenized to make nanosuspension by utilizing sonicator. Molecule Size Conveyance, X-Beam Diffraction (XRD), Immersion Solvency, Disintegration Rate, Soundness Test, pH impact, Checking Electron Microscopy (SEM), Differential Filtering Calorimetry (DSC), Medication Delivery Profile Review and Fourier Change Infrared Spectroscopy (FTIR) portrayals were performed for nanosuspensions. Created nanosuspension had incredible way to deal with further develop home grown drugs solvency and improved bioavailability.

Keywords: Nanosuspensions, Sono-precipitation, Molecule Size Conveyance, Immersion Solvency, Disintegration Rate,

MSNANO-23 (71)

Ultrafast Monitoring of Toxic Pollutant Arsenic In Water Via 3-D Nano-Pyramids metal oxide/polymer Based Electrochemical Sensor Encapsulated In Porous Carbon Material.

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Abstract

Novel nanocomposite cobalt oxide with poly (3, 4- ethylenedioxythiophene)-polystyrene sulphonate (PEDOT) have been synthesized for the detection of Arsenic ions in the aqueous solution. The structural features of the material have been characterized by field emission scanning electron microscopy, XRD, Raman, thermogravimetric and differential thermal analyses. Cyclic voltammetry at potential range −0.2 to 0.05 V from aqueous NaOH solution (pH 7) produced a well-defined cobalt oxide PEDOT nanocomposite deposition on glassy carbon electrode(GCE) surface. Cobalt oxide PEDOT nanocomposite based GCE has shown excellent electrocatalytic activity towards virulent inorganic arsenite in micromolar and nanomolar concentrations present in real water samples. The current-time amperometric response for the detection of arsenic shows reliable and reproducible results with correlation factor 0.9991. Differential pulse voltammetric technique has also been utilized for the evaluation of newly fabricated electroanalytical sensor. This shows excellent catalytic activity toward arsenic oxidation at wide alkaline pH range, exhibited good selectivity and lower limit of detection upto 10nM. In comparison with the other electrochemical procedures, fabricated GCE electrode offers remarkable sensitive signals, long term reliability, good reproducibility, and simple procedure with a lower detection limit.

MSNANO-23 (72)

EFFECT OF DIVALENT DOPANT ION, ON DIELECTRIC AND ABSORPTION PROPERTIES OF TB3+, DY3+ CO- DOPED SPINEL FERRITES

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Abstract

Ferrites are materials, which are extensively used in electronic, electrical and magnetic applications. Among ferrites, spinal ferrites are more efficient ones because of their excellent properties like tunable dielectric constant, excellent thermoelectric behavior and high saturation magnetization. To enhance novel properties of spinal ferrites, in this research work we have investigated the effect of nature of divalent dopant ion (M=Co, and Ni) on rare earth (RE3+ = Dy3+and Tb3+) co-doped spinel ferrites. The samples doped by different metals like NiFe1.8Tb.06Dy.14O4 and CoFe1.8Tb0.6Dy0.14O4 has been successfully prepared by using sol-gel auto-combustion method. And a base sample Fe3O4 has been synthesized adopting same route, to compare the different parameters of metal ions doped samples. The formation of nano-scale particles was confirmed by XRD reflections. XRD and scanning electron microscope were used to investigate structural and morphological properties of prepared samples. XRD reflections confirmed the phase purity and single phase of FCC structure development of all synthesized samples. Crystallite size was found to be increasing, as, 19.39 (nm), 25.07 (nm) and 40.18(nm) for Fe3O4, NiFe1.8Tb.06Dy.14O4 and CoFe1.8Tb0.6Dy0.14O4 respectively. And lattice constant was found to be decreasing as from 8.44 Å, 8.41 Å and 8.37 Å respectively for all synthesized samples. Thermal properties of synthesized samples were investigated by using Seebeck apparatus. The dielectric studies revealed that with increase of frequency, the dielectric constant and dielectric loss both decreases and approaches to zero with further increase in frequency

MSNANO-23 (73)

First principle investigations on Magnesium Oxynitride for electronic, thermoelectric, and optical applications

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Abstract

Metal oxynitrides are promising research candidates for modern electronic devices due to their superior thermoelectric, and optical characteristics. In this work, nitrogenized magnesium oxide was investigated through density functional theory calculations for the prediction of the electronic, thermoelectric, and optical responses. The density of states spectra revealed the significant contribution of Mg-s, and O-p states for pristine MgO, while N-p states provide maximum contributions with overlapping at the Fermi level in nitrogen- containing compositions. The calculated band gap of pure MgO using the TB-mBJ approximation corresponded well with reported theoretical and experimental results. The bandgap of pure and N-doped MgO compositions observed to reduce with the increment in nitrogen concentration. The thermoelectric properties of pure and N doped MgO compositions were evaluated using Boltz Trap code and showed significant variations after doping. A sharp increase in optical parameters especially the absorption coefficient in the visible region was observed with an increment of nitrogen content. Epsilon near zero response was recorded in compositions containing more than 6.25% nitrogen which makes these advantageous for tunable electronic devices.

MSNANO-23 (74)

EFFECT OF MAGNETIC FIELD ON GERMINATION AND SEEDLINGS OF SPINACH (SPINACIA OLERACEA L.)

Farah Naz

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Abstract

To overcome food insecurity, it is essential to increase production in agriculture crop in developing nations. Now a days different techniques are used to enhance seed performance and crop yield, electromagnetic fields is one of them which is an important and useful tool. The

researchers are willing to try to increase agricultural output and seed germination by employing a variety of ways to improve their growth performance. The objective of present work was to study the pre-sowing magnetic field influence on plant growth, plant germination, and shoot length, the length of the root, and sprouting growth, and development as well as the biological properties of spinach. The present research work comprises the investigation of the effect of a magnetic field on spinach seeds. For this purpose, the spinach seeds were treated with a magnetic field at electromagnetic lab department of physics UAF. Untreated seeds were used as a control. The non-uniform full wave rectified magnetic field was used to treat the seeds of spinach with varying intensity of time. Flat plot in the vegetative area of Institute of Horticultural Sciences was selected for the field experiment at the University of Agriculture Faisalabad. The treated and non-treated seeds were planted in this area with three replicates. It was found that the magnetic field affected a number of physical and biochemical variables, including seed germination. The collected results were evaluated using statistical techniques to find out the differences between the untreated and treated seeds. Magnetic treatments boosted the spinach's growth and characteristics.

MSNANO-23 (75)

SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL APPLICATIONS OF SCHIFF BASES DERIVED FROM THIOSEMICARBAZIDE

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Abstract

Schiff bases are important medicinal organic compounds that play significant role in pigments, dyes, catalysts, intermediates in organic reactions and are also known to exhibit various biological activities. Three different thiosemicarbazide containing Schiff bases 1-(4-hydroxy-3-

methoxybenzylidene) (HTSC), 1-(3-methoxybenzylidene) (MTSC), and 1-(3-isopropylbenzylidene) (PTSC) were synthesized and characterized by using FTIR, ¹H NMR, ¹³C NMR and crystal XRD. These compounds' structures were optimized computationally using Gaussian 09W to evaluate several geometrical and quantum mechanical parameters. Geometrical parameters that were calculated were also compared to calculated values and were found to be in good agreement. Using BR buffers, the electrochemical response of all the synthesized compounds was investigated over a broad pH range. Moreover, the lipid profile, blood cell morphology and in vivo antidiabetic activity of these compounds were screened. Thus, Schiff bases and their derivatives may be further used for enormous biological applications with potent effects.

Keywords: Schiff bases, Spectroscopy, X-ray analysis, Computational analysis, Voltammetric characterization, Antidiabetic activity.

MSNANO-23 (76)

Fuel Performance Comparison of Uranium Nitride and Uranium Carbide in VVER-1200 using OpenMC

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Abstract

Nuclear power is a reliable and large-scale source of GHG-free electricity. This study assesses the viability of ATF fuel of uranium nitrate (UN) and uranium carbide (UC) as fuel for the VVER-1200 reactor. A comprehensive overview of the VVER-1200 and Accident Tolerant fuels

is conducted. A review of the development of ATFs identified UN and UC as viable fuels for the VVER reactor. The study utilizes OpenMC to model the VVER-1200 core and compares the behaviour of ATF with conventional fuel. Key findings include comparable k-eff values implying similar neutronic behaviour. UO₂and UC showed similar fission rates across the core while UN showed higher neutron flux and fission rate in the outer part of the core. The base Z44B2 showed increased flux and fission rate with UN as the fuel. ATF behaviour showed to be comparable to the UO2 and thus is a potential alternative to conventional fuels. ATFs provide an additional level of safety because of higher melting points and higher thermal conductivity. This study can be further improved to investigate the depletion of ATFs so that the behaviours of the core over large periods of time, fission products and operator safety can be assessed. Base case k-eff value of 1.24795 are comparable to k-eff values generated by UN and UC.

MSNANO-23 (77)

Effects of Water-Flow Rates on Structural and Diffusion Properties of Carbon Nanotubes

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Abstract

Molecular Dynamics (MD) Simulations has been used to determine the structural analysis and diffusion coefficients of armchair single walled carbon nanotubes (SWCNTs) filled with water. It has been demonstrated that how different physical parameters i.e. flow rates v(m³/s) and temperature T(K) affect the structure and

diffusion of armchair SWCNTs. Computer software Material Studio has been used for modeling the structures of water molecules and armchair SWCNTs, and LAMMPS has been employed along with appropriate mathematical models and potentials to calculate diffusion coefficients with varying parameters, T(K) and v(m³/s). Radial distribution functions (RDFs) has been computed to examine the SWCNTs which is considered to be an appropriate tool for structural analysis. In addition, powerful three dimensional softwares, Visual Molecular Dynamics (VMD) and Open Visualization Tool (OVITO) have been used to visualize the complete picture of nanotube structure. It has been shown that the obtained results for diffusion coefficients of SWCNTs from MD methods are found in satisfactory agreement with earlier known numerical MD results.

MSNANO-23 (78)

Synthesis and charchterization of chromium metal with pyromellitic acid

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Abstract

Three coordination complexes of chromium metal were synthesized with pyromellitic acid ligand.Different synthetic techniques like sonication, reflux and stirring were explored.Effects of co-ligand, solvent choice, metal ligand molar proportion and pH were also studied.The charachterization of metal complexes was done by FT-IR, photo-Luminescence and UV-Vis spectroscopic methods.FT-IR spectra confirmed the shifting of peaks of metal complexes and free ligand which indicate coordination.%Quenching of metal complex 1 against potassium dichromate was 35%. The photocatalytic activity of metal complexes was evaluated against methylene blue and the degradation pattern were compared under dark and sunlight.Metal complex 2 and metal complex 3 showed degradation activity 90% and 79% respectively .

MSNANO-23 (79)

Study of Karpman Washimi magnatization in solid state plasma

Rehan Ullah

Department of Physics, GCU Lahore

Abstract

Three coordination complexes of chromium metal were synthesized with pyromellitic acid ligand.Different synthetic techniques like sonication, reflux and stirring were explored.Effects of co-ligand, solvent choice, metal ligand molar proportion and pH were also studied.The charachterization of metal complexes was done by FT-IR, photo-Luminescence and UV-Vis spectroscopic methods.FT-IR spectra confirmed the shifting of peaks of metal complexes and free ligand which indicate coordination.%Quenching of metal complex 1 against potassium dichromate was 35%. The photocatalytic activity of metal complexes was evaluated against methylene blue and the degradation pattern were compared under dark and sunlight.Metal complex 2 and metal complex 3 showed degradation activity 90% and 79% respectively .

MSNANO-23 (80)

RP-HPLC Method for identification and quantification of 5-Fluorouracil released from cross linked chitosan nanoparticles using Human and Rabbit Plasma Samples

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Abstract

The objective was developed and validation of a simple, accurate, precise, cost effective and sensitive reversed phase high pressure liquid chromatography (RP.HPLC) method for determination of 5-fluorouracil (5-FU) in human and rabbit plasmas by ethical approval committee with reference number 29-2017/PREC. 5-FU is a broad spectrum anticancer and it is widely used in the treatment of various types of solid cancers. But due to its narrow therapeutic window, plasma concentration is very essential to determine at clinical setups. Therefore the current RP-HPLC chromatography system is developed and it is an isocratic of Agilent technologies series 1200 consisted of a pump and variables. Data processing software ChemStation used with a Wave length Detector (VWD) for assay of prepared plasma samples. Mobile phase composition was acetonitrile: water (10:90) at pH 6 and 1.0 mL/min flow rate for 3-4 minutes (retention time). 5-Fluorouracil was detected using a Waters 2996 photodiode array

detector at a 260 nm wavelength. The calibration curve was linear over the concentration range of 2-100ng/ml. This method was specific and co-relation coefficient (r2) is less than or equal to 0.998. It is concluded simple and reproducible method may be employed for the analysis of pharmacokinetic parameters, in both rabbit and human plasma samples.

MSNANO-23 (81)

Harvesting water from atmosphere using metal-organic framework

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Abstract

By 2050, nearly half of the world's population is estimated to live in water-stressed regions due to arid conditions or lack of access to clean water. Plenty of water can be harvested from the desert atmosphere, where the humidity is low, and from more humid regions where clean water is needed. In principle, the materials used to harvest water from air in these climates should apply to deployment anywhere worldwide to extract atmospheric water at any time of the year. Metal–organic frameworks (MOFs) have emerged as a unique class of porous materials capable of trapping water from the atmosphere at very low relative humidity (up to 10 % RH) conditions and releasing it at relatively moderate temperatures (60 oC). For this purpose, the zirconium-based metal-organic framework MOF-801 was synthesised. XRD analysis reveals that the average crystallite size of MOF is 38.87 nm, whereas most are 20-30 nm, as measured by SEM. When exposed to controlled 20% RH conditions, the 115 g of MOF-801 captured 33 mg of water in six hours.

MSNANO-23 (82)

Effect of electric field intensity on the desalination of brackish water by capacitive deionisation

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Abstract

Due to rapid industrialisation, climate change, population explosion and the spread of water pollution, natural freshwater resources can no longer meet the growing global demand for clean water. Seawater and brackish water with abundant reserves cannot be directly used as domestic water. Therefore, brackish water desalination is one of the most effective solutions to overcome clean water shortages. One of the major drawbacks of all the existing water desalination technologies (thermal distillation, reverse osmosis (RO), and electrodialysis (ED)) is their high energy requirements. Therefore, there is a dire need to develop an energy-efficient desalination technology to fulfil an ever-increasing clean and fresh water demand.

In a capacitive deionisation (CDI) cell, a DC voltage is applied across two porous electrodes separated by a narrow channel of brackish water. In this work, the porous electrodes were fabricated by activated carbon powder. The effect of the intensity of the electric field on the removal of salt (NaCl) ions from brackish water was determined by varying the electric potential difference from 1.5 V to 3 V across the electrodes separated by a water channel of 2 cm width.

The results show that at a constant flow rate (i.e., 20 mL/min) of brackish water between the electrodes, the removal rate of salt ions increased with increasing the electric field intensity. During the 2.5 hours of CDI experiments, five litres of brackish water was desalinated, and its salt concentration decreased from 250 mg/L to below 100 mg/L. The maximum salt removal efficiency of 62% was achieved under the applied electric field of 1.5 V/cm. The preliminary results show that CDI is a promising technology for brackish water desalination.