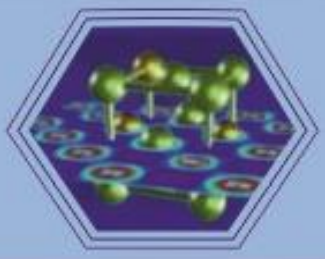
TEERTHANKER MAHAVEER UNIVERSITY, MORADABAD
FACULTY OF ENGINEERING & COMPUTING SCIENCES

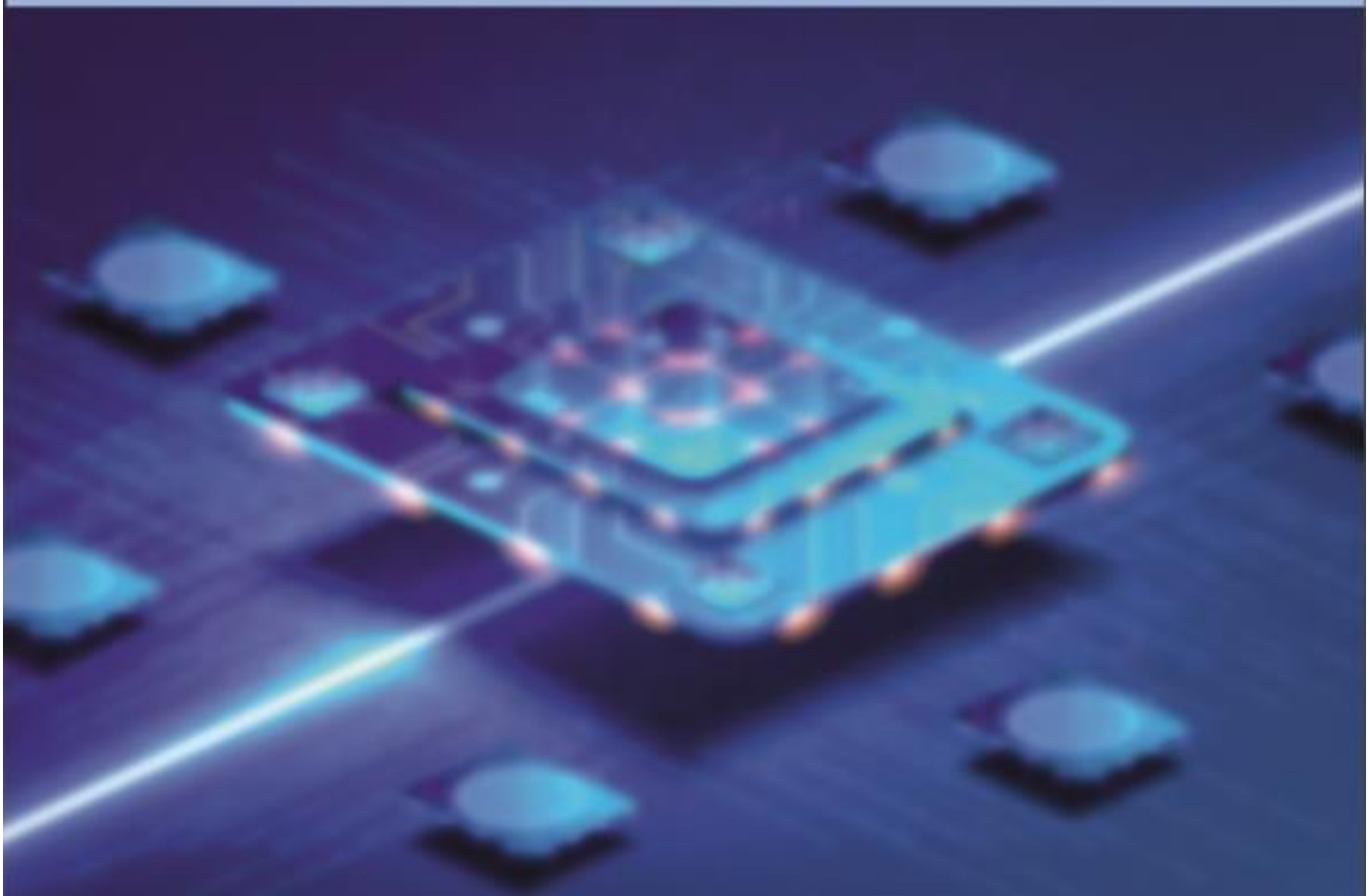
DEPARTMENT OF PHYSICS



NATIONAL CONFERENCE ON

NCMD 2020

MATERIALS & DEVICES



DR. AMIT. K. SHARMA : HEAD, PHYSICS
PROF. S. P. PANDEY : CONVENOR
DR. PAVAN K SINGH : SECRETARY
PROF. RAKESH KR. DWIVEDI : CONFERENCE GENERAL DIRECTOR

Supported By :

MESSAGE BOARD

Hon'ble Chancellor: Shri Suresh Jain

The pillars of Teerthanker Mahaveer University (TMU), Moradabad are laid on the quintessence of academic pursuit and excellence which, we believe can be actualized with uttermost allegiance, hard work, and diligence. TMU is poised to become a Centre of Excellence in Academics and Research. Research and development, needless to say, forms the backbone of our curricula. In this untiring strife, every college of the university is involved in various path-breaking innovative research activities all throughout the year by putting into place conferences and seminars every so often on contemporary and relevant topics with an aim to expedite research in those areas which will lead to indispensable metamorphosis in the academia as well.
Faculty of Engineering & Computing Sciences (FoE & CS) has, to its credit, a matchless stature in UP and the country altogether by breaking new grounds in producing professionals of national and international acclamation and has been acknowledged as one of the top ranking institutions offering high quality education. With the commitment of highly qualified and efficient staff, the college endeavours enthusiastically to make mark in the field of research and development by setting up an ambient academic environment for its students and research scholars.
I congratulate Prof. R. K. Dwivedi, Director & Principal FoE & CS & Team of Department of Physics for his all-time unwavering efforts and wish the conference a great success. It is my humble wish that this professional dialogue and collaboration among the researchers, engineers, students and educators will linger and prosper for many years to come.
Kudos Team NCMD-2020!

Hon'ble Vice –Chairman: Shri Manish Jain

I am very glad to know that the Faculty of Engineering & Computing Sciences, Teerthanker Mahaveer University, Moradabad, is going to organize a National Conference in Materials and Devices "NCMD-2020" supported by IEEE UP section from 18th - 19th December, 2020. Conferences are great way for academicians to b e inspired by fresh ideas to start rethinking the status kuo, and to hopefully leave ready to tackle academic challenges in inspired and innovative ways. Conferences also allow individuals to share their progress, hurdles they have come across, and technical devices for solving them. I am also glad to know that even the pandemic could not dampen the zeal enthusiasms of our academicians and students. I hope that the conference achieves its objectives and I also extend my best wishes for a great success of NCMD-2020.

Esteemed Member of TMU Society: Shri Akshat Jain

I would like to congratulate FoE & CS for organising the National Conference in Materials and Devices "NCMD-2020" from 18th -19th December, 2020. The aim of the conference is to provide of global platform for academicians, researchers and Scientists coming from various National Institutes/ Universities and Research Laboratories to present their breakthrough facts, research findings and innovations in the field of material science and their devices. I hope that this conference serves as a platform for exchanging the views and ideas among national participants. I would like to express my appreciation to the organizing team for their hard work and relentless efforts. I extend my best wishes for the grand success of the conference.

Hon'ble Vice-Chancellor

Faculty of Engineering & Computing Sciences has, to its credit, a matchless stature in UP and the country altogether by breaking new grounds in producing professionals of national and international acclamation and has been acknowledged as one of the top ranking institutions offering high quality education. With the commitment of highly qualified and efficient staff, the college endeavours enthusiastically to make mark in the field of research and development. It is heartening that the Department of Physics, College of Engineering and Computing Sciences, Teerthanker Mahaveer University, Moradabad is going to organise **National Conference on Materials and Devices (NCMD-2020)** on 18 – 19th Dec.-2020. This national conference on materials and devices will be very helpful to setup an ambient academic environment for its students and research scholars. The Department fraternity deserves all praise for its commendable, collective and collaborative efforts which is poised to bring about quality transformation in the perception and personality of all participants through discussion deliberation and conclusion at the conference.

I extend my hearty congratulations and good wishes to all concerned for the smooth and successful conduct of the conference.

Registrar: Dr. Aditya Sharma

I am heartily elated to know that FoE & CS, Teerthanker Mahaveer University, Moradabad UP, India is going to organise NCMD-2020, the National conference on materials and Devices from 18th- 19th, December, 2020. I am confident that the conference would set fire to the learning and academic achievements of national researchers & academicians by providing a stage for intellectual conversation and deliberate in the field of Physics of Materials and Devices. I am sure that the conference would pave the way of scientific involvement to the fields of scientific creativity.

Conference General Chair: Prof. Rakesh Kumar Dwivedi

Greetings! We at Faculty of Engineering &Computing Sciences & Information Technology (CCSIT) Teerthaker Mahaveer University Moradabad, extend a hearty invitation to all our academic fraternity colleagues to take a part in National Conference on Materials and Devices (NCMD-2020).

The relationship between institutions and industry is highly synergetic. Since the primary objective of students in pursuing higher education in the area of Science, Engineering Computer Applications & Animation, is to get a good career on completion of their studies, the institutions need the support of industry and research institution to help the scholar's in academic nurturing process. On the other hand, the industry looks towards institutions for their requirement of qualified and

trained professionals. Thus, it is in the interest of both Industry & Institutions to develop strong cooperation, which can be win-win for both, and will also be beneficial to the students and research scholars.

This has been the guiding principle for us at FoE& CS, that we want our scholar's/students to be a good professional in their defined domains. Hence we conduct extensive Employability Enhancement Training Program, Seminars, workshops and conferences designed to develop skills and provide value-added training and certifications in their respective domains. They are also getting exposer through practical aspects of the industry via guest lectures, industrial visits, projects and internships etc.

FoE & CS highly appreciate the confidence reposed in us and the invaluable support extended by author's and key note speakers.

Department of Physics, FoE& CS TMU Moradabad is committed to ensure the best discussion and deliberations experience amongst all delegates and assure you of our best efforts. **Happy NCMD-2020!**

Dr. Amit Kumar Sharma,
Head, Department of Physics, FOE & CS, Teerthanker Mahaveer University, Moradabad

Greetings!

As a Head of Physics, I take great pride in welcoming all the attendees of the National Conference on Materials and Devices - 2020. This conference is dedicated to researching and fighting for the development of new devices as a part of the current scenario. On behalf of the Department of Physics, I welcome you to NCMD-2020, and wish you a successful conference. It is hoped that NCMD-2020 will be a platform to gather and disseminate the latest knowledge in recent advancements in emerging areas of diversified research fields covered during this conference. Academicians, Scientist, Researchers will be able to share and discuss new findings and applications of Materials in the devices. It is envisaged that the intellectual discourse will result in future collaborations between universities, research institutions and industry both locally and nationally.

Convenor- NCMD-2020: Prof. S.P. Pandey

We cordially invite you to attend and submit your abstract and papers for the our National Conference on Materials and Devices (NCMD-2020)" which is going to be held on December 18-19, 2020 at Department of Physics, Faculty of Engineering and Computing Sciences.

This national conference on materials and devices (NCMD-2020) is to support research community by empowering Professor, Scientists, Researchers, Students and Business Delegates to regularly meet and discuss topics with frontrunners in the field of materials and their recent findings. Materials and its applications in form of devices have always played a key role as one of the main pillars of economic progress and social well-being in any country and indeed the world as a whole. The challenges encountered in the research problems and to explore the possibilities of the new collaborators with top academicians and scientists from the field of materials and their applications in the form of devices is also be the theme of this conference.

We believe that this conference would have one good aspect for sharing of knowledge and providing the platform to explore the innovative learning for new researchers in their respective area of research interest.

TEERTHANKER MAHAVEER UNIVERSITY, MORADABAD
FACULTY OF ENGINEERING & COMPUTING SCIENCES

National Conference on Materials and Devices (NCMD-2020)

18 & 19 December, 2020)

NATIONAL CONFERENCE ON NCMD2020 MATERIALS & DEVICES

Organized by
Department of Physics
Faculty of Engineering & Computing Sciences
Teerthanker Mahaveer University
Moradabad-244001

PROGRAMME SCHEDULE

Day – 1 (18th Dec.-2020; FRIDAY)		
Timings (Indian Standard Time)	**EVENTS**	**Total Time**
Zoom Meeting Link	https://zoom.us/j/93417769155?pwd=WUdYWEgxYmdUR2ZLY29KUExpSkVOUT09	
10:00 to 11:00AM	**Inaugural Function**	60 Minutes
10:00 - 10:05 AM	**Lighting the lamp Ceremony (Saraswati Vandana)**	05 minutes
10:05 - 10:15 AM	**Welcome Address:** Prof. R.K. Dwivedi, Director-FOE & CS, Theme Elaboration	10 minutes
10:15 - 10:20 AM	**Welcome Address :** Dr. Aditya Sharma**,** Registrar TMU, Moradabad	05 minutes

10:20 - 10:30 AM	**Address:** Prof. Raghuvir Singh, Vice-Chancellor-TMU, Moradabad			10 minutes
10:30 - 10:40 AM 10:40 - 10:50 AM 10:50 - 10:55 AM	Chief Guest : Dr.D.K. Avasthi **(Former Scientist-IUAC)** Prof. R.K. Shastri, Vice Chancellor Gurukul Kangri Vishwavidyalay, Haridwar Guest of Honour : Prof. Mukul Kishore (Hindu College, Moradabad)			10 minutes 10 minutes 05 minutes
10:55 - 11:00 AM	Address : Prof. S.P. Pandey (Convener)			05 minutes
Session-1 (11:00AM – 1:00PM)				
	(Session Chair: Dr. Kamlesh Pandey)			
11:00 - 11:35 AM	**Keynote Address**	Prof. S. A. Hashmi University of Delhi, New Delhi	Biomass-based Eco-friendly Carbon Electrodes for Solid State Supercapacitors	30 + 5 = 35 Minutes
11:35AM – 12:00 PM	**Plenary Talks-1**	Dr. Bhaskar Bhattacharya Department of Physics, MMV, BHU, Varanasi	Polymer Electrolyte Based Solar Cells : PEC to QDSC	20 + 5 = 25 minutes
12:00 – 12:20 PM	**IT-1**	O. M. Hussain *Thin films Laboratory, Dept. of Physics, Sri Venkateswara University, Tirupati*	Carbonaceous transition metal oxide nanocomposites for high performance energy storage devices	15 + 5 = 20 minutes
12:20 – 12:40 PM	**IT-2**	Dr. Nidhi Asthana *National centre of Experimental Mineralogy and Petrology, University of Allahabad*	Spectroscopic Study on Compatibility of PVB (poly-vinyl butyral) With Organic Solvents	15 + 5 = 20 minutes
12:40 – 1:00 PM	**IT-3**	Dr. R.J. Deokate *Department of Physics, V P Arts Science and Commerce College, Baramati, Pune*	Advanced Nano Material Synthesis by Spray Pyrolysis Technique	15 + 5 = 20 minutes
Session-2 (1:45PM – 4:30PM)				
		(Session Chair: Dr. Nitin A. Jadhav)		
1:45 – 2:10 PM	**Plenary**	Dr. D.K. Rai	Probing ion transport in polymer electrolytes using	20 + 5 =

	Talks-2	*Jaypee Institute of Information Technology, Noida*	FTIR spectroscopy	25 minutes
2:10 – 2:30 PM	**IT-4**	Rajeev Sehrawat, *Department of Physics Maharishi Markandeshwar University (MMDU), Mullana, Ambala*	Effect of oxidizing agents on polpyrrole capped carbon coated $LiFePO_4$ cathode material for Lithium ion battery	15 + 5 = 20 minutes
2:30 – 2:50 PM	**IT-5**	Dr. Madhulata Shukla *Department of Chemistry,* *G.B. College, Ramgarh, Kaimur, Veer Kunwar Singh University,* *Bihar, India*	Ionic Liquids: A superior Solvent for Synthesis and Stabilization of Metal nanoparticles	15 + 5 = 20 minutes
PARALLEL ORAL SESSION-1 (Session Chair: Dr. Diptonil Banerjee)				
Zoom Meeting Link	https://zoom.us/j/93417769155?pwd=WUdYWEgxYmdUR2ZLY29KUExpSkVOUT09			
3:00 – 3:10PM	**O-1**	Anju Bala, *Department of Physics Maharishi Markandeshwar deemed to be University (MMDU), Mullana (Ambala),India*	Effect of polyaniline capping on the Optical Properties of $ZnS_{/Mn}$ Quantum Dot	8 + 2 = 10 Minutes
3:10 – 3:20PM	**O-2**	Ms. Abha *Dr. A. P.J. Abdul Kalam Technical University, Uttar Pradesh, Lucknow*	Synthesis and Developement of Cellulose Based AloveraNanocomposites Membrane for Food Packaging	8 + 2 = 10 Minutes
3:20 – 3:30PM	**O-3**	Dr. Diptarka Roy *Department of Physics, BabasahebBhimraoAmbedkar (Central) University, Lucknow*	Synthesis of polyvinyl alcohol (PVA)- Polyaniline (PANI) composite membrane for electrochemical devices	8 + 2 = 10 Minutes
3:30 – 3:40PM	**O-4**	Sanjay R. Kale *Post-graduate Department of Chemistry TuljaramChaturchand College Baramati Pune*	Synthesis and Characterization of Rare Earth doped Y_2O_3Phosphor Material	8 + 2 = 10 Minutes
3:40 – 3:50PM	**O-5**	B. S. Maharnavar *V P K B I Engg. and Technol.,*	Effect of Rare earth element Doping on	8 + 2 = 10 Minutes

		Baramati. Pune	Structural and Magnetic Properties of Ni-Co mixed spinel Nanocrystalline Ferrites	
3:50 – 4:00PM	**O-6**	*Areeb Alam,* Department of Physics, TMU, Moradabad	Graphitic Carbon Nitride as Water Purifier: A Review	8 + 2 = 10 Minutes
4:00 – 4:10PM	**O-7**	Himanshu (Rathore) *Nanostructures Engineering and Modeling Lab, Metallurgical Engineering and Material Sciences Department, IIT Bombay, Mumbai, Maharashtra, India-400076*	Synthesis and Characterization of Graphene-Composite Foam	8 + 2 = 10 Minutes
4:10 – 4:20PM	**O-8**	Sudeep Kumar Das *Department of Physics, DurgapurGovernment College J. N. Avenue, Durgapur, PaschimBardhaman, West Bengal*	Scaling Exponents in 2+1 Dimension for Random-Ballistic Competitive Growth Model	8 + 2 = 10 Minutes
4:20 – 4:30PM	**O-9**	Dr. Sananda Jana *Department of Physics (BSH)* *Techno International Batanagar Maheshtala, Kolkata-141 West Bengal, India*	Photo-switching Behaviour of Chemically synthesized Lead Sulphide multi armed Dendritic crystals	8 + 2 = 10 Minutes
4:30 – 4:40PM	**O-10**	Pawan Singh Dhapola *Nano Science and Nano Technology Center, Dept. of Chemistry, Kumaun University, Nainital, Uttarakhand* *Material Research Laboratory, School of Basic Sciences & Research, Sharda* University	Synthesis of highly conducting ionic liquid incorporated polymer electrolyte and porous carbon material for efficient supercapacitor	8 + 2 = 10 Minutes
4:40 – 4:50PM	**O-11**	Jeevitesh K Rajput, *Department of Physics, Babasaheb Bhimrao Ambedkar University, Lucknow, India*	Recent development and challenges in Zinc oxide (ZnO) based Gas Sensors	8 + 2 = 10 Minutes
PARALLEL ORAL SESSION-2 (Session Chair: Dr. L. K. Tiwari)				

Zoom Meeting Link	https://zoom.us/j/96572834685?pwd=SnRmS1BhUG5oYXlzNHdsdEozVTIyQT09			
3:10 – 3:20PM	**O-12**	Anoop Kumar Pandey *Department of Physics K S Saket P G College Ayodhya*	Geometry optimization vibrational frequencies electronic properties of Urecil Mustred by using DFT	8 + 2 = 10 Minutes
3:20 – 3:30PM	**O-13**	Vijay Singh *The University of Dodoma, Dodoma (Tanzania)*	DFT study of superhalogen properties YCl_n(n=1-6) complexes	8 + 2 = 10 Minutes
3:30 – 3:40PM	**O-14**	Jyoti Kapil *Department of Physics, AIAS, Amity University, Noida, Uttar Pradesh, India.*	DFT Study of Structural, Electronic and magnetic properties of Half-metallic Full- Heusler Alloy Ru_2VSb	8 + 2 = 10 Minutes
3:40 – 3:50PM	**O-27**	Mohd. Kamran, *Department of Physics, Faculty of Engineering,* *Teerthanker Mahaveer University, Moradabad, India*	A REVIEW ON THERMODYNAMIC ASPECTS OF BULK METALLIC GLASSES AND THEIR APPLICATIONS	8 + 2 = 10 Minutes
3:50 – 4:00PM	**O-28**	Kailash Kumar Yadav, *Department of Physics, Teerthanker Mahaveer University, Moradabad*	Study on Irradiated and Hydrogenated metal-Semiconductor Devices	8 + 2 = 10 Minutes
4:00 – 4:10PM	**O-29**	Nirmal Kumar Verma *Department of Physics, Shri Jai Narain P.G. College, Lucknow.*	Third harmonic radiation generation by propagation of laser beams in under dense plasma	8 + 2 = 10 Minutes
4:10 – 4:20PM	**O-30**	Gaurav Mishra *Department of Physics K S Saket P G College Ayodhya*	Biological AIM analysis Fukuai Function caculation of Urecil Mustred by First Pincipal	8 + 2 = 10 Minutes
4:20 – 4:30PM	**O-31**	Vinod Kumar Singh	An investigation Superacidic properties of	8 + 2 = 10

		Department of Physics K S Saket P G College Ayodhya	hydrogenated FeF_n^-(n=1-6): A DFT study	Minutes
4:30 – 4:40PM	**O-32**	Prashant Singh *Department of Physics Rajendra College Chhapara Bihar*	DFT study of Bioactive Agent - Proflavine	8 + 2 = 10 Minutes
4:40 – 4:50PM	**O-37**	Deshraj Singh *Department of Physics K.G.K. College, Moradabad*	Study of Stability and Protonic Conductivity of Composites Electrolytes $(1-x)CsH_2PO_4/xZrO_2$ For Fuel Cells	8 + 2 = 10 Minutes

Day – 2 (19th Dec.-2020)

SESSION – 3 (9:50AM – 1:00PM)

Timings (Indian Standard Time)		**EVENTS**		Total Time
Zoom Meeting Link	https://zoom.us/j/93417769155?pwd=WUdYWEgxYmdUR2ZLY29KUExpSkVOUT09			
Address : Dr. Manjula Jain, Associate Dean –Academics				
(Session Chair: Dr. Amit Saxena)				
10:00 to 10:35AM	**Keynote Address**	Prof. Neelam Srivastava Department of Physics, MMV, BHU, Varanasi	Conductivity-Power-Law and ion dynamics	30 + 5 = 35 Minutes
10:35 - 11:00 AM	**(Plenary Talks)**	Prof. U.P. Singh KIIT, Bhubneshwar	Thin Film Solar Cell Technologies: Current Status and Future Prospects	20 + 5 = 25 minutes
11:00 - 11:20 AM	**IT-6**	Prof. P.K. Singh *SBSR, Sharda University*	Ionic Liquid Doped Solid Polymer Electrolyte for Dual Energy Devices	15 + 5 = 20 minutes

11:20 - 11:40 AM	**IT-7**	Sunil Kumar Pandey, *Department of Physics, Nims University Rajasthan, Jaipur*	STUDIES ON HYDROGEN ABSORPTION/ DESORPTION BEHAVIOURS OF $La(NI_{0.80}Fe_{0.20-X}Mn_X)_5$ ALLOYS	15 + 5 = 20 minutes
11:40AM - 12:00 PM	**IT-8**	N. Yedukondalu *Department of Geosciences, Center for Materials by Design, and Institute for Advanced Computational Science, State University of New York, Stony Brook, 11794-2100, NY, USA*	Materials design by crystal structure prediction methods and its applications	15 + 5 = 20 minutes
12:00 - 12:20 PM	**IT-9**	Remyamol T. *Vikram Sarabhai Space Centre*	Mechanical, Thermal and Electrical Properties of Hot-Pressed Graphite/Silicon Carbide composite – An insight to the anisotropic behavior and high heat flux applications	15 + 5 = 20 minutes
12:20 - 12:40 PM	**IT-10**	Mukta Tripathi, *Department of Physics, Marwadi University, Rajkot-360005, Gujarat, India*	Past, present and future of energy storage devices	15 + 5 = 20 minutes
12:40 – 1:00 PM	**IT-11**	Dr. G.N. Pandey *Department of Applied Physics, Amity Institute of Applied Sciences, Amity University, Noida,*	Metamaterials: Fundamentals and Applications	15 + 5 = 20 minutes
SESSION – 4 (1:45PM – 4:15PM)				
(Session Chair: Prof. Asim Ahmed)				
1:45 - 2:10 PM	**(Plenary Talks)**	Prof. N.B. Singh SBSR, Sharda University	Green method of synthesis of nanomaterials and their applications	20 + 5 = 25 minutes
2:10 - 2:30 PM	**IT-12**	Harish Kumar *Department of Physics, Nims University Rajasthan, Jaipur, INDIA*	Enhancement in hydrogenation behaviours by Going Off Stoichiometry in Ti-V based alloy tailored with excess Ti	15 + 5 = 20 minutes

2:30 - 2:50 PM	**IT-13**	Dr. Meenal Gupta *Department of Physics, Material Research Laboratory, School of Basic Sciences & Research, Sharda University, Gr. Noida 201310, India*	Carbon based electrode materials for Supercapacitors	15 + 5 = 20 minutes
2:50 - 3:10 PM	**IT-14**	Yogesh Kumar* *Department of Physics, ARSD College University of Delhi, New Delhi-110021, India* *(*Corresponding author Email: ykumar@arsd.du.ac.in)*	NANO-STRUCTURED ACTIVATED CARBONS AS ELECTRODE MATERIAL FOR HIGH PERFORMANCE ELECTROCHEMICAL SUPERCAPACITORS	15 + 5 = 20 minutes
PARALLEL ORAL SESSION-3 (Session Chair: Dr. Vishnu Prasad Srivastava)				
Zoom Meeting Link	https://zoom.us/j/93417769155?pwd=WUdYWEgxYmdUR2ZLY29KUExpSkVOUT09			
3:10 – 3:20PM	**O-15**	Usman Yusuf Bello *Material Research Laboratory, Department of Physics, Sharda University, Greater Noida, Uttar Pradesh, India*	High Conducting PVDF-HFP+PTA polymer electrolytefor Supercapacitor application	8 + 2 = 10 Minutes
3:20 – 3:30PM	**O-16**	Arnab De *Department of Industrial & Applied Chemistry, Swami Vivekananda Research Centre, Ramakrishna Mission Vidyamandira, Belur Math, Howrah-711202, India*	Enhanced Photoluminescence properties of Na^{+} co-doped $SrAl^{2}O^{4}$: Eu^{3+} chain like nanophosphor for solid state lighting application	8 + 2 = 10 Minutes
3:30 – 3:40PM	**O-17**	Ankita Chandra *[a]School of Materials Science and Nanotechnology,*	Improved photocatalytic activity of Zinc Cadmium Sulfide under Visible Light Irradiation	8 + 2 = 10 Minutes

		Jadavpur University, Kolkata 700032		
3:40 – 3:50PM	**O-18**	Shital Prasad *J C Bose University of Science and Technology, YMCA , Faridabad, Haryana, India*	Optical properties of Al-doped ZnO Thin Film deposited by Sol–Gel route	8 + 2 = 10 Minutes
3:50 – 4:00PM	**O-19**	Suvra Pal *Department of Physics, Jadavpur University, Kolkata 700032, India*	Realization of theoretically predicted cold electron emission from oxide perovskite: vanadium doped $BaSnO_3$ nanocubes	8 + 2 = 10 Minutes
4:00 – 4:10PM	**O-20**	Brahami Das *Department of Physics, Hooghly Mohsin College, Chinsurah, Hooghly 712101, India*	Morphology modulated Ga_2O_3 nanostructures for green water purification technology	8 + 2 = 10 Minutes
4:10 – 4:20PM	**O-33**	Rajeev Sehrawat, Anju Bala *Department of Physics, MMU, Mullana, Ambala*	Synthesis of polyvinyl alcohol (PVA) capped ZnS nanosize particles: structural and morphological properties	8 + 2 = 10 Minutes
4:20 – 4:30PM	**O-34**	HARSH *Department of Physics, MMU, Mullana, Ambala*	HARTREE FOCK ELECTRONIC STRUCTURE STUDIES OF RITALIN AND CAFFEINE	8 + 2 = 10 Minutes
4:30 – 4:40PM	**O-35**	Aveensh Mishra *Future Institute of Engg. & Technology, Bareily*	Low Frequesct Electrical Behaviour of a Fluorinated Liquid Crystalline Material with Many Phases	8 + 2 = 10 Minutes
PARALLEL ORAL SESSION-4 (Session Chair: Dr. Parag Agrawal)				
Zoom Meeting Link	https://zoom.us/j/96572834685?pwd=SnRmS1BhUG5oYXlzNHdsdEozVTIyQT09			
3:10 – 3:20PM	**O-36**	Brahma Prakash Dubey *Department of Physics, Indian Institute of Technology Roorkee, Uttarakhand-India*	Microstructural Influenced Conduction Mechanism of Mn-doped Garnet type Solid Ionic Conductor	8 + 2 = 10 Minutes
3:20 – 3:30PM	**O-21**	Sudarshan Sarkar *Indian Institute of Technology (BHU), School of Materials*	Doped g-C_3N_4 : an Efficient Water Purifier	8 + 2 = 10 Minutes

		Science and Technology, Varanasi, India		
3:30 – 3:40PM	**O-22**	Jitendra Gaur *BRCM College of Engineering & Technology, Bahal (Bhiwani)- Haryana 127028*	Thermodynamical study of Oxide glass forming melts	8 + 2 = 10 Minutes
3:40 – 3:50PM	**O-23**	R. R. Awasthi, *Department of Physics, University of Lucknow, 226007, India*	Fabrication of bismuth ferrite multiferroic lead-free high T C ferroelectric material	8 + 2 = 10 Minutes
3:50 – 4:00PM	**O-24**	SHUBHAM *Department of Physics, MMEC, MMU, MULLANA (AMBALA) – 133207 (HARYANA) INDIA*	COMPARISON OF EUGENOL AND PAPAIN - A REVIEW	8 + 2 = 10 Minutes
4:00 – 4:10PM	**O-25**	P. Das, *School of Material Sc. & Nanotechnology, Jadavpur University, Kolkata 700 032, India*	Tuning transport properties of $CuBO_2$ via sulphur doping	8 + 2 = 10 Minutes
4:10 – 4:20PM	**O-26**	Azemtsop Manfo T *Department of Physics, MRL, SBSR, Sharda University, Greater Noida 201 310, India*	PVDF-HFP + NaSCN and Ionic liquid based polymer electrolyte for supercapacitor	8 + 2 = 10 Minutes
4:20 – 4:30PM	**O-38**	Pawan Kumar *Department of Physics, Gurukula Kangri University, Haridwar*	Electrical Conductivity and Thermal Analysis of CsH_2PO_4(CDP)/NaH_2PO_4(SDP)/ZrO_2 Composites Electrolyte for Fuel Cell	
4:30 – 4:40PM	**O-39**	Ratna Sarkar, Department of Physics, Jadavpur University, Kolkata, India	PVP varied BiOCl nano-crystals effective Photocatalytic Performance by Rhodamine B dye degradation under visible light	8 + 2 = 10 Minutes

4:40 – 4:50PM	**O-40**	***Narbir Singh***[a,b], *Kamalika Banerjee*[b], *Yogesh Kumar*[a]*	Performance of choline chloride based electrolytes in electrochemical double layer capacitors	8 + 2 = 10 Minutes

Valedictory Function (4:20PM – 4:25PM)

Zoom Meeting Link :

https://zoom.us/j/93417769155?pwd=WUdYWEgxYmdUR2ZLY29KUExpSkVOUT09

Vote of Thanks & A brief report on National Conference NCMD-2020

(Presented By Convener of the Conference)

National Advisory Committee

Prof. S. A. Hashmi (University of Delhi)

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Key-Note-1

Biomass-based Eco-friendly Carbon Electrodes for Solid State Supercapacitors

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In recent years, a world-wide attention has been devoted to develop electrochemical supercapacitors for their potential application as alternative power sources to the rechargeable batteries in various applications e.g. computer power backup, medical equipment, load leveling in electrical vehicles (EVs), space crafts, etc. These devices are attractive due to their increasing demand having high specific power and durable cycle life (10^5-10^6 cycles) for various applications. The supercapacitors namely electrical double layer capacitors (EDLCs) with large area carbon electrodes attract the consumers due to their robust nature, ability of large-scale production and lower cost.

In this presentation, main focus is devoted towards carbon supercapacitors based on polymer-based electrolytes. Fundamentals of supercapacitors would be briefly described first in terms of the electrode and electrolyte materials, charge storage mechanisms and their various configurations. Emphasis would be given to solid-state devices using polymer based electrolytes, recently developed in our laboratory. It is well known that supercapacitors offer lower specific energy as compared to rechargeable batteries, although the power density is substantially high. Current issue of supercapacitor development is associated with the increase in their specific energy. Some important and recent studies on carbon supercapacitors based on biomass-derived activated carbon and gel polymer electrolytes, carried out in our laboratory, would be presented.

Key-Note-2

Conductivity-Power-Law and ion dynamics

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The frequency dependence of conductivity indicates that ion movement changes from hopping to correlated hopping and then goes to caged motion of ion, as we move towards higher frequency. The observation of any of these in particular range is just a matter of statistical dominance of the phenomenon in that specific frequency range. Many empirical and theoretical efforts are made to understand the behavior. The mathematical representation of conductivity and frequency relationship came into existence when Jonscher in 1976 analyzed a large amount of data and presented them as $\sigma= \sigma_0 + A\omega^n$, with the restriction on exponent 'n' to have value approximately between 0.55 to 0.65, irrespective to the morphology of systems and type of charge carriers. Latter when data became available in wider frequency and temperature range it has been recognized that the above law deals with hopping/ correlated hopping ion transport only and for caged motion of ion the value may be >1 also, and a modified formula which is later known as super-linear-power law has been given as $\sigma= \sigma_0 + A\omega^n + B\omega^m$ where $n<1$ and $m>1$. Many theoretical attempts have been made to explain the behavior of exponent 'n' with temperature and salt concentration, but exact theory has still to be developed. Depending upon the system exponent 'n' is found to have positive or negative slope with temperature, which requires explanation. Our group has carried out a systematic analysis of data on different polymeric systems and explained the variation of exponent with temperature and salt concentration. In polymeric systems depending upon salt concentration, material is divided into two groups salt-in-polymer and polymer-in-salt and they have different ion transport mechanism. Proper analysis of conductivity formalism also differentiate between these two categories, and even the analysis in salt-in-polymer range can give an indication that whether the particular combination of polymer and salt will result in polymer-in-salt type of systems at higher salt concentration or not. The conductivity-law analysis with $\tan\delta$ Vs frequency analysis can be used to develop a detailed understanding of the ion dynamics of any system. The developed analysis process is not limited to polymeric systems, it is equally applicable to other ion conducting systems also.

Plenary Talk-1

Polymer Electrolyte Based Solar Cells : PEC to QDSC

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Polymer electrolytes are widely explored and used due to their various advantageous properties, such as ability to form thin films, flexibility, light weight, elasticity, high ionic conductivity etc. For last 4 decades polymer electrolytes have been widely used in electrochemical devices like solid state rechargeable batteries, fuel cells, supercapacitors and electro-chromic display devices and solar cells. The last one is the least explored one so far.

In literature, it was reported that addition of natural salts to polymers (insulating polymers) modifies their properties and the resulting polymer salt complex achieves high ionic conductivity which is desirable for good device performance. However, the environmental compatibility remains as a challenge for majority of such polymer electrolytes. Use of bio-polymers as electrolyte is one of the simple and interesting route. The bio-derived polymers can simply be modified by doping with suitable salts which can provide ions for transport. Depending upon their physical parameters, one can obtain a dry polymer electrolyte film or form gel of desired thickness. Accordingly, the conductivity and ion transport gets affected and altered.

This talk shall be focussed on the use of polymer electrolytes in various solar cells. Initial works on photoelectrochemical solar cells (PEC), which established the fact that polymer electrolytes **can** really work in solar cells, indicated variety of problems. The 3rd generation solar cells, dominantly the Dye sensitized solar cells (DSSCs), have been fabricated with different polymer electrolytes. Inorganic polymers modified by doping, blending, addition of fillers have shown promising results. The possibilities of doping with ionic liquids have also been explored. Use of bio-polymers have also been tested which made the devices environment friendly. The recent developments using Quantum Dots and Perovskites in conjunction with polymer electrolytes as solar cells shall also be discussed. Attempts shall be made to frame a possible guideline for choice of optimum polymer electrolytes.

Plenary Talk-2

Probing ion transport in polymer electrolytes using FTIR spectroscopy

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For more than two decades, polymer electrolytes have drawn global attention for their development and applications in electrochemical devices like batteries, fuel cells, supercapacitors, etc. Due to their excellent electrochemical properties and solid state consistency, these electrolytes are replacing conventional liquid electrolytes as an alternative for more compact and improved energy storage devices. Mouldability, flexibility, low temperature processibility, thin film formability of polymer electrolytes make them special among the available choices of electrolytes for device applications.

Polymer electrolytes, generally, are the materials in which a macromolecular matrix (polymer or polymer blend) is incorporated with salts. This polymer-salt combo processed normally as films/ membranes offer a significantly good ionic conductivity. For ion transport in polymer electrolytes, coordination of constituents like interaction of polymers in the blends, and coordination of ion with the polymer matrix plays a major role.

Infrared spectroscopy is an important technique which probes material structure at molecular level. The unique vibrational bands of infrared spectra result from vibrational motions of individual bond or groups in a molecule. Any change, therefore, occurring in the bonding situations of molecules results in the change in vibrational frequency. In this presentation, results of FTIR studies carried out on few polymer electrolyte systems will be discussed

Plenary Talk-3

Thin Film Solar Cell Technologies: Current Status and Future Prospects

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Today the PV market is dominated by the well established poly and single crystalline Si products. Polycrystalline thin film technologies offer further cost reduction potential for PV, as well as new product configurations such as light-weight and flexible modules. Thin film solar cells and modules, however, suffer from certain limitations caused by the polycrystalline nature of the semiconductor absorber layers used in the device structures. Manufacturing experience for thin film modules is also rather limited. Despite these difficulties, thin film technologies based on Cadmium Telluride (CdTe) and Copper Indium Gallium Selenide (CIGS) polycrystalline absorber layers showed great advancement during the last decade. Small area CIGS and CdTe solar cells demonstrated conversion efficiencies of nearly 23% and 22%, respectively. A world record efficiency of 20.4% on polyimide film has also been achieved recently, revealing that flexible solar cells with performance close to rigid solar cells can be developed. The CIGS solar cells may limited by the long term availability of In and CdTe suffered due to the involvement of toxic Cd and the availability of Te. The world attention has shifted to more environmental friendly and abundant material CZTS (Copper Zinc Tin Sulfide) and it has made a steady progress with time. The main advantage of this cell over CIGS solar cells are low production cost and the replacement of the expensive Indium (In) by less expensive Tin (Sn) and Zinc (Zn). The highest efficiency achieved at lab scale for CZTSe and CZTSSe is 12.6% and 11.1% respectively. In this presentation the review of the development of polycrystalline thin film PV technologies, their present status and future prospects will be discussed.

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Plenary Talk-4

Green method of synthesis of nanomaterials and their applications

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Abstract

Nanotechnology has become one of the most promising technologies applied in all areas of science. However, most of the chemical methods involved in the preparation of nanomaterials are expensive and involve the use of toxic chemicals that pose various biological risks. Therefore, the alternative methods, which are less toxic, eco-friendly and in-expensive are being explored. The nanotechnology industry is increasingly promoting nano as a green technology that will improve the environmental performance of existing industries, reduce consumption of resources and energy, and allow achievement of environmentally benign economic expansion. Synthesis and characterization of nanoparticles are important steps to be adopted to apply nanoparticles in field applications. To synthesis stable metal nanoparticles with controlled size and shape, there has been search for inexpensive, safe, and reliable and green approach. The novel methods so called green/biosynthesis have been recently developed by a variety of plant extracts and microbes. In this paper numbers of plant extracts and microbes have been used to synthesize nanomaterials and their applications have been discussed.

Invited Talk-1

Carbonaceous transition metal oxide nanocomposites for high performance energy storage devices

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Abstract:

The fast growing demand for sustainable energy has triggered intense research in design and development of advanced energy storage devices. Supercapacapatteries represent a major technology to store energy for many applications including electronics, automobiles, hybrid vehicles, military, and space. The supercapattery can possess energy as much as the battery and output power almost as high as the supercapacitor because of hybridization of the merits of supercapacitor and battery. The efficiency of the supercapattery is mainly depends on the class of electrode materials and their microstructure and electrochemical properties. The advent of carbonaceous transition metal oxide nanocomposite (CTN) materials has spurred enormous research interest as supercapattery electrode materials due to their fascinating electrochemical properties. In the present work, the cutting-edge research on development of carbonaceous nanocomposite materials- various synthesis approaches, tuning of microstructure, electrochemical performance etc., for achieving high energy and power densities are discussed.

Keywords: Supercapattery • Transition metal oxides • Carbonaceous nanocomposites •

Invited Talk-2

Spectroscopic Study on Compatibility of PVB (poly-vinyl butyral) With Organic Solvents

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Abstract

The study deals, the versatile behaviour of poly vinyl butyral (PVB) and we aimed at finding different solvents for PVB and determine the effect of solvents. PVB is a low –cost alternative, showing flexibility, optical clarity and good adhesion to many surfaces. The random structures of PVB result in glassy polymers with no discernible crystallinity except at very high alcohol content. The chain contains both hydrophilic vinyl alcohol groups and hydrophobic (or less hydrophilic) vinyl butryl groups. The most important to choose the PVB as the host polymer is that PVB has been used in laminated glass for over 60years due to its high stability against sunlight without degradation in its transparency or adhesion to glass. The implementation of ionically conductive PVB film as a solid state electrolyte film for electrochromic devices (ECDs) have been reported.PVB polymer have been extensively used in many applications science. PVB is a low cost alternative showing flexibility, optical clarity and good adhesion to many surface, as well as excellent mechanical strength and impact resistance. substantial amount of unreacted vinyl alcohol units typically remain in the chain and so PVB is best regarded as a random co-polymer of vinyl butryl and vinyl alcohol unit the vinyl alcohol unit is polar and hydrophilic and the vinyl butryl is hydrophobicthe hydroxyl and acetate group acts as promoter of polymer adhesive in the glass surface. The relative proportion of the hydroxyl group, acetate group and acetal groups are controlled by the condition of the acetal reaction. The non polar, polar and hydrogen bonding components of PVB can interact favourably with other macromolecules and it may therefore be compatible with both hydrophilic polymers and hydrophobic. It is soluble in different polar solvents like Acetic Acid, DMF, THF and Ethenol. The miscellanies of all the solvents THF, Ethenol and DMF respectively along with the Acetic Acid, with maintaining their distinct ratios, are very efficient to produce PVB membrane. The polar solvents have also been used for improving the electrical conductivity of the polymer. Polar solvent vapour treatment was reported as a better method. . The conventional solution cast technique has been used for the preparation of solid polymer membrane based on PVB. A ratio, of (95:5) PVB and solvents was annexed individually with 20 ml of different solvents such as DMF, THF, Acetic Acid and Ethenol

respectively. After annexation of the solvents with PVB, the mixtures were kept under constant stirring for 5 hours, using Revotek magnetic stirrers (Germany). Then, the solutions were poured in petri dishes and dried in constant humidity and temperature condition. Structural behavior of pure PVB, polymer electrolyte films with different solvents and different annealing temperatures were studied by X-ray diffractometer (Phillips X-Pert model). The SEM images of different electrolyte systems were recorded with JEOL JXA-8100 EPMA instrument. The infrared spectrum was recorded on Brucker Alpha (Germany) FTIR with ATR spectrophotometer in a range 4000-500cm^{-1}. FTIR spectrum of same sample annealed at various temperatures was recorded. Raman spectra were collected with Uniram confocal Raman spectrophotometer with laser sources at 785nm with variable power in the spectral range (0-2000 cm^{-1}).

Invited Talk-3

Advanced Nano Material Synthesis by Spray Pyrolysis Technique

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Abstract:

Presently in fundamental scientific areas and many more technological fields are centered on functional nanostructured materials due to their unique physical and chemical properties. Supercapacitors are the favorable energy storage and conversion device with high energy and power density. Chemical spray pyrolysis (CSP), deals with substantial potential for preparation of numerous nanostructured materials with tailorable composition and morphology. Furthermore, growth control properties have glowed the researcher as compared to solid state reaction process or other chemical method. The various functional nanostructured materials can be synthesized by CSP for the application in energy storage and conversion. Here we have reported change in structural, morphological results with change in various parameters of CSP. The different form thin films, hollow structures, core shells, nanoplates, Nanorods and different composites are presented. Lastly, few challenges of CSP for the preparation of nanostructured materials are discussed.

Keywords: Thin film, Chemical spray pyrolysis, Nanostructure, nanorod, etc.

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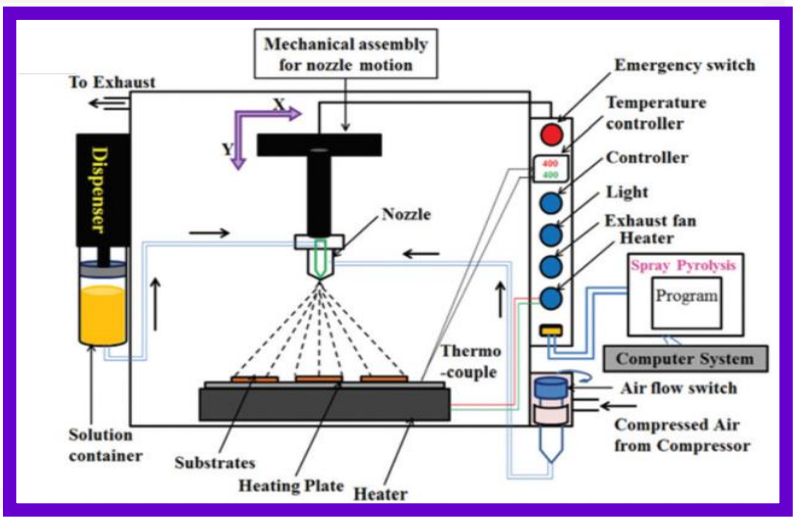

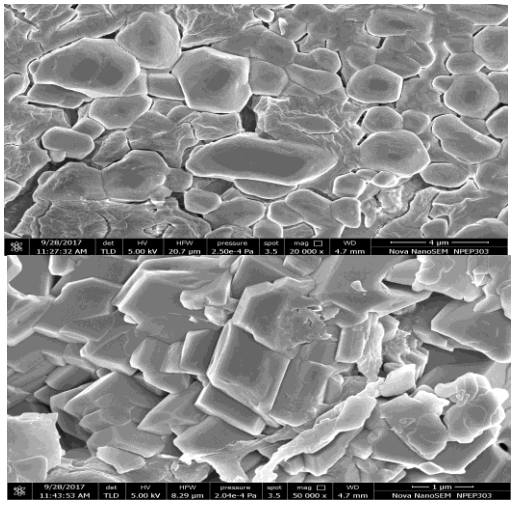

Invited Talk-4

Effect of oxidizing agents on polpyrrole capped carbon coated $LiFePO_4$ cathode material for Lithium ion battery

Rajeev Sehrawat[a], Rashmi Mittal[a], Anil Kr. Sharma[a], M.K. Bera[a], S.P. Panday[b]

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Keywords: ***polypyrrole****, lithium iron phosphate, Discharge capacities,* H_2O_2

Polypyrrole coated lithium iron phosphate (LFP/C-Ppy) composite materials were synthesized by in-situ polymerization. $KMnO_4$ (strong) and H_2O_2 (weak) oxidizing agents were used to polymerize the pyrrole monomers on $LiFePO_4$/C particles. The estimated polymer content in the composite material was 6.4 and 5.4 wt%. for oxidizing agent $KMnO_4$ and H_2O_2 respectively, while the carbon content was estimated as 8wt.% in LFP/C material, using thermogravimetric analysis. SEM determines the particles size 200 nm of synthesized $LiFePO_4$/C material. The particles of LFP/C-Ppy composite materials were well agglomerated via the surface Polypyrrole and a slight increment in the particles size was estimated due to the Polypyrrole coating as confirmed by FESEM micrographs. The phase analysis of LFP/C was performed using X-ray diffraction, which confirms the pure single phase of $LiFePO_4$. For the composite materials LFP/C-Ppy, the peaks belong to, $LiFePO_4$ and $Li_{0.05}FePO_4$ along with low intensity impurity peak of $Fe_2P_2O_7$ when synthesized using $KMnO_4$ oxidizing agent. But the impurity peak corresponding to $Fe_2P_2O_7$ was not observed in the pattern and a pure single phase $Li_{0.5}FePO_4$ appeared in the diffraction pattern of LFP/C-Ppy composite using H_2O_2 oxidizer. Discharge capacities of 145 and 134mAh/g were obtained at 0.1C rate, for LFP/C-Ppy composite materials synthesized using H_2O_2 and $KMnO_4$ oxidants respectively, while the discharge capacity of 139mAh/g was obtained for LFP/C at this current rate. The deterioration in the capacity for the composite material synthesized using $KMnO_4$ was due to impurity phase $Fe_2P_2O_7$ as observed in the X-ray diffraction pattern.

Invited Talk-5

Ionic Liquids: A superior Solvent for Synthesis and Stabilization of Metal nanoparticles

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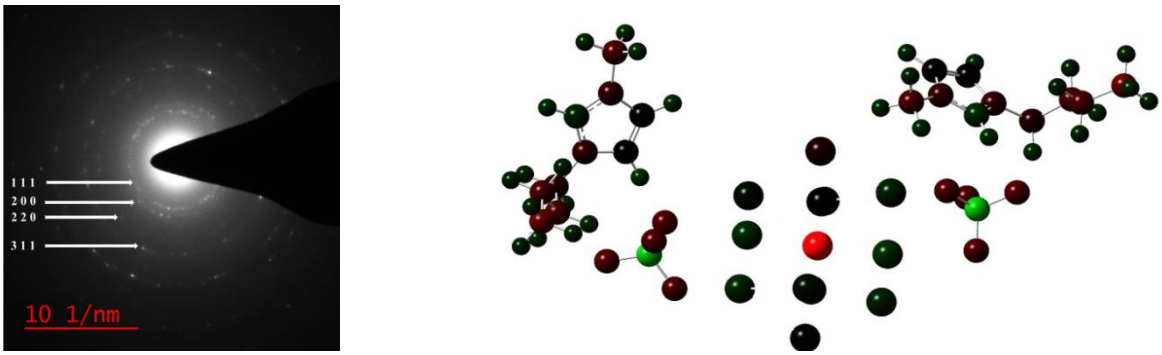
Abstract:

The mechanism of stabilization of silver nanoparticles (AgNPs) by 1-butyl-3-methylimidazolium tetrafluoroborate ionic liquid (IL) is elucidated from experimental spectroscopic investigations and density functional theory (DFT) calculations. FTIR spectrum of the synthesized IL stabilized silver nanoparticles reveals small red shift in B-F stretching frequency while C-H stretching remains unshifted. There is no shift in NMR peaks of IL before and after the synthesis of IL stabilized Ag NPs. This suggests that Ag NPs are surrounded by anions of ILs. The optimized structure obtained from density functional theory (DFT) calculations also shows the anionic part of the IL surrounding the Ag nanocluster. This is supported by the IR frequency data calculated using DFT. The calculated interaction energy obtained between cluster and IL is considerably attractive. Density of State (DOS) calculation shows that the HOMO-LUMO gap of the Ag cluster-IL composite is significantly lesser than that of the IL alone.



(i) (ii)

Figure (i) Electron diffraction pattern of synthesized Ag NPs (ii) NBO charge distribution on Ag13-2bmimBF4 (Red colour represents the most electronegative element and green colour represents the electron deficient atom) indicating that BF4 ions are much closer to the Ag 13 cluster.

Invited Talk-6

Ionic Liquid Doped Solid Polymer Electrolyte for Dual Energy Devices

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Abstract

Solid electrolyte are attracted researchers due to various advantageous properties like no leakage, no corrison, no evaporation etc. Albeit their low ionic conductivity always play a main barrier. In recent years low viscosity Ionic liquids (IL) mixed with polymer electrolyte seems best candidate as an electrolyte material in energy devices [1-3]. Veriety of low viscosity ionic liquid, like 1-ethyl -3-methyl imidazolium dicynamide (EmImdcn, viscosity 28 cP at 20 $^{\circ}$C) and a polymers, *i.e.* polyvinyl alcohol (PVA), Polyethylene oxide (PEO) have been prepared using solution cast technique and characterized by impedance spectroscopy, optical microscopy (OM), differential scanning calorimetry, x-ray diffraction (XRD), and fourier transform infrared spectroscopy (FTIR). Mixing ionic liquid with polymer matrix supresses the crystallinity of polymer matrix and enhancement in electrical conductivity was noted. Finally we have tested these IL doped high conducting solid polymer electrolyte films in energy devices namely supercapacitors and dye sensitized solar cell.

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Invited Talk-7

STUDIES ON HYDROGEN ABSORPTION / DESORPTION BEHAVIOURS OF $La(NI_{0.80}Fe_{0.20-X}Mn_X)_5$ ALLOYS

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ABSTRACT

We have investigated Fe and Mn substituted version of $LaNi_5$ i.e. the alloys $La(Ni_{0.80}Fe_{0.20-x}Mn_x)_5$ by material tailoring. It has been found that all the phases of $La(Ni_{0.80}Fe_{0.20-x}Mn_x)_5$ exhibit better hydrogenation characteristics than the parent material $LaNi_5$/$La(Ni_{0.80}Fe_{0.20})_5$. The storage capacity of $La(Ni_{0.80}Fe_{0.20-x}Mn_x)_5$ for x = 0.20, 0.06, and 1.0 are 1.95, 1.98 and 2.0 wt% at 50^oC respectively. The material $La(Ni_{0.80}Fe_{0.20-x}Mn_x)_5$ has been found to exhibit the highest storage capacity ~2.0 wt%. This is again one of the high storage capacity observed for AB_5 type material at ambient conditions. We will therefore, describe here the substitution of Mn for Ni/Fe. Detailed investigations of $La(Ni_{0.80}Fe_{0.20-x}Mn_x)_5$ for x = 0.10 revealed that the material $La(Ni_{0.80}Fe_{0.20-x}Mn_x)_5$ exhibits the highest storage capacity ~2.0 wt%. It is about 33% higher than the capacity of the parent alloy $LaNi_5$ (~1.5 wt %). We have also studied the thermodynamic aspect, effect on plateau pressure, and change in lattice parameter and unit cell volume with Mn substitution in place of Ni/Fe.

The aim of the present work is to see the effect, which factor are more responsible for enhancement in hydrogen storage capacity i.e. electron attractive power or atomic size of the substituted element by materials taoloring.

- Presenting Auther

Keywords: Hydrogen storage alloy; Pressure–composition–isotherms.

Invited Talk-8

Materials design by crystal structure prediction methods and its applications

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Abstract:

Crystal structure prediction (CSP) methods have shown tremendous success during the last decade in discovering novel (structural and functional) materials for diverse applications namely high Tc-superconductors, superhard, thermoelectric materials and many more. Universal Structure Predictor: Evolutionary Xstallography (USPEX) based on the evolutionary approach is one of the most successful CSP methods (which is developed by Prof. Artem R. Oganov from Russia) [1]. USPEX is an open source, widely used with many functionalities and very user friendly. In the present talk, I will briefly describe the methodology and recent developments of USPEX [2], and its application for prediction of hidden martensite phase transition in MClF (M = Sr, Ba and Pb) compounds under high pressure [3].

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Invited Talk-9

Mechanical, Thermal and Electrical Properties of Hot-Pressed Graphite/Silicon Carbide composite –An insight to the anisotropic behavior and high heat flux applications

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Abstract:

Dense, homogenous and EDM machinable Graphite-SiC composites of two different compositions were developed by simple hot pressing of the homogenized powders under vacuum at 2125 ^{o}C and 30 MPa load. The applied unidirectional load resulted in the orientation of graphite flakes resulting in highly anisotropic properties. The materials were characterized using XRD, FESEM and Raman analysis. FESEM analysis clearly indicates the ordering of the hexagonal graphite flakes in the hot pressing direction. The anisotropy in mechanical, thermal and electrical properties of hot pressed graphite/SiC composites are studied in detail. The material is also tested in the plasma arc jet facility at a simulated heat flux of 750 W/cm^2 and shows no erosion, hence a potential material for nozzle throat inserts of motors of launch vehicles.

Invited Talk-10

Past, present and future of energy storage devices

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Abstract:

In recent few years energy storage devices attracted wide interests of researchers. Basically two devices widely used in the market battery and supercapacitors. Various researcher developed energy storage device supercapacitors using various biomass based activated carbon as electrode materials, nanocomposite polymer electrolytes for achieving higher power density. Batteries attracted peoples interest due to higher energy density of the device. We need to Developed of Hybrid energy storage device Supercapattery for High energy density and high-power density. Hybrid storage device supercapattery, which essentially combines a battery electrode (faradaic material) and a supercapacitor electrode (non-faradaic material). For this purpose, the various materials and the techniques have been utilized to enhance the charge storage of the device. Various characterization related to battery and supercapacitors has been required to find out the various properties. In Future that hybrid device is used in various automobiles and gagets.

Invited Talk-11

Metamaterials: Fundamentals and Applications

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Abstract-

In 1967, Veselago [1] first considered the case of a medium that had both negative dielectric permittivity and negative magnetic permeability at a given frequency and concluded that the medium should then be considered to have a negative refractive index (i.e. the negative square root, $n = -\sqrt{\varepsilon\mu}$). S.A. Ramakrishna [2] has examined the problem of making materials with negative material parameters which are mostly structured composites. The design of meta-materials that show a negative refractive index is an extreme form of electromagnetic engineering. The left-handed materials (LHMs) also called negative index materials (NIMs) or double negative (DNG) materials are artificial composite with both negative permittivity ε and permeability μ. In this invited talk, I discuss about the optical properties, band structures and dispersion relation of one dimensional photonic crystal (1-D PC). I also discussed about the fundamental of metamaterials and its application by using translational matrix method (TMM). Metamaterial Photonics Crystal is the 1-D PC containing negative index materials is a periodic arrangement of positive index material (PIM) and negative index material (NIM).

Key Words: *Photonic Crystals, Left –handed materials (LHMs), Negative index materials (NIMs),*

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Invited Talk-12

Enhancement in hydrogenation behaviours by Going Off Stoichiometry in Ti-V based $_{alloy}$ tailored with excess Ti

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Abstract

The present paper describes and discusses enhancement in hydrogenation behaviour of $Ti_{0.85}V_{0.95}Fe_{0.15}Zr_{0.05}$ alloys going off stoichiometry in Ti which is known to be promising candidate of Ti-V system of alloys hydrogen storage. It has been found that by taking excess of Ti corresponding to $Ti_{0.85+x}V_{0.95}Fe_{0.15}Zr_{0.05}$ (x = 0.02, 0.03, 0.04, 0.05 and .06) leads to enhancement of plateau pressure upto 2.5 atmosphere at 100 ^{o}C. Also the excess Ti alloy gets activated easily and starts absorbing significant hydrogen from the very first cycle. The present studies suggest that instead of foreign elements, variation in stoichiometry of one of the native elements may be more effective for making the hydrogen storage material amenable for devices.

Keyword: Hydrogen storage alloy**;** Pressure–composition–isotherms; Cyclic stability; Laves phases

Invited Talk-13

Carbon based electrode materials for Supercapacitors

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Abstract

Now a days clean energy generation is prime concern for any developed country to maintain global effects. Battery is still the main product of the market even through its discard is not very easy for environment concern. Electrochemical capacitors are alternative of batteries but it need lots of efforts by reseachers to imrove its performance according to industrial need. Electrochemical double layer supercapacitor (EDLC) has its two main components: electrode and electrolyte. Most of the EDLCs are based on porous carbon materials [1-4] used as electrode material. Due to high surface area of porous carbon, such supercapacitor have high specific capacitance but their low density is also responsible to decrease the gravimetric capacitance. Therefore to improve the gravimetric capacitance high density carbon materials are required to use them as electrode material. Recent literature [5-6] confirms that non porous carbon materials show utra-high capacitance. Nonporous carbon based on Polyvinylchloride (PVC) has been developed. Using Brunauer–Emmett–Teller (BET), the calculated value of surface area ~ 1.19 m_2/gm. These electrode materials are compatible with imidazolium based electrolyte materials which shows high gravimetric capacitance. In this talk, I will present current status of non-porous carbon as well as porous carbon based electrodes and ionic liquid (IL) based electrolyte to develop efficient EDLC.

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Keywords: carbon electrodes, ionic conductivity, ionic liquid, supercapacitors

Invited Talk-14

NANO-STRUCTURED ACTIVATED CARBONS AS ELECTRODE MATERIAL FOR HIGH PERFORMANCE ELECTROCHEMICAL SUPERCAPACITORS

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In this rapidly changing world in this post-modern era, according the report of United Nations, there are three major challenges before the world now a day: 1) Energy, 2) water, 3) Security. The nano-carbons address the two major challenges. Nano carbon powders, carbon nanotubes (CNTs), have been studied for the energy storage/conversion and capacitive deionization applications. There are few excellent results based on these materials has been reported [1-5]. The cost of de-ionizing agents is always a major challenge in industrial applications. In the search of indigenous sources, Humic acids (HA) extracted from peat and HA derived nano-carbon has been studied by solid-state nuclear magnetic resonance spectroscopy (NMR) with magic angle spinning, thermal decomposition study using mass spectroscopy, differential scanning calorimetry (DSC), thermo-gravimetric analysis (TGA), Raman spectroscopy and the method of standard contact porosimetry (MSCP). The composite of HA derived carbon (HADC) with graphene oxide (GO) has been prepared using in-situ carbonization of HA in the presence of graphene oxide in an inert atmosphere at 900 °C. As a result of carbonization of HA, small agglomerates of carbon with sharply defined edges has been obtained, and the composite of HADC-GO forms only a large aggregates. The value of specific surface area of HADC and HADC-GO composite carbonized at 900 ^{o}C are 3 and 237 m^2/g, respectively. There are various issues related to physics at nanoscale as far as capacitors concerned with nanocarbons.

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Invited Talk-15

Structure Texture and Marphology Modulation of mesoporous elcctrode for effecient sensitized solar cells

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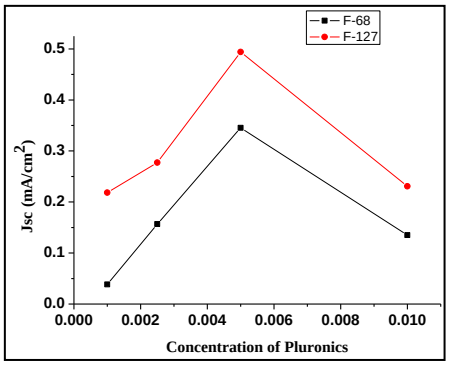
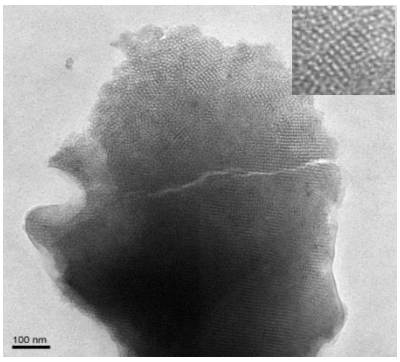
Wide band gap semiconductors like TiO_2, ZnO are used as working electrode for dye-sensitized solar cell (DSSC), in present study highly ordered nanoporous TiO_2 and ZnO materials with crystalline frameworks were successfully synthesized from different concentration of triblock co-polymer (soft templates) like F-127 F-68. Synthesized mesoporous TiO_2 have variation of pore size ranging from 2-5 nm and having high specific surface area from 216 m^2/g to 352 m^2/g. A photoelectrode fabricated using synthesized mesoporous TiO_2 shows increase in photocurrent (Jsc) with increase in pore size as well as surface area and change in Voc with variation in structure texture and morphology of photoelectrode. The sensitized solar cells were fabricated using N3 dye as well as alkyl ammonium lead halide (Perovskite) sensitizers and solid polymer electrolyte with KI/I_2 as redox electrolyte. Synthesized samples were characterized by XRD, TEM, and Brunauer- Emmett-Teller (BET). Photovoltaic performance of DSSC overall conversion efficiency (%), fill factor (FF), open-circuit voltage (V_{OC}) and short-circuit current (I_{SC}) from the I–V curves measured with 2400 Keithley Source meter, it was observed that the photoelectric performance is strongly dependent on combined effect of Voc and Jsc which shows the characteristic change with structure texture morphology as well as pore size and specific surface area of fabricated electrode.





Invited Talk-16

Recent Development in Polymer Electrolytes for Rechargeable Batteries

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Abstract

In the series of development in electrochemical cells, rechargeable batteries are the most popular identity. where the device not only providing energy to the electrical equipment but can be charged again. in 1990, the first rechargeable battery was introduced and commercialized by the Japanese company Sony. still, there is a lot to work required to comeover the limitations, like energy density, leakage, and flammability. To overcome these limitations researchers and scientists are working for over three decades. in this aspect, the major development was reported for electrolytes. where initially the liquid electrolytes were replaced with solid electrolytes and to compensate for the conductivity of liquid electrolytes, much work has been done in the enhancement in the conductivity of these solid electrolytes. In this direction, the development of solid polymer electrolytes with high ioinic conductivity and good chemical and mechanical stability for application in various electrochemical devices has been an impotrant area of research in the past few decades. For electrode application and also for better compatibility with the electrolyte, the research on mixed conductor (ionic+electronic) is focussed.

It is possible to develop a mixed conductor by controlled doping the same host polymer which is (generally) used as electrolyte. Keeping above fact in mind Poly (ethylene oxide) PEO, complxed with NaI (Salt), is adopted as a host polymer for the further doping of Si/C_{60}/CuI to develop the mixed conduting polymer, that can be used as the electrode material in batteries.

Present talk shall be focussed on the electrical characterization for C_{60} dispersed composite polymer electrolyte thin films. The polymer films were prepared at different wt% of dispersoid.The host polymer

electrolyte matrix is of (PEO: NaI) at fixed cation to monomer ratio. Here, $C_{60}$was prepared in laboratory and has been verified with NMR data sheet. Further, the prepared samples were subjected to structural and electrical characterization. The composite nature of the films is verified with the X-ray diffraction and FTIR. The CISwas used to study the electrical conductivity of the films. The polarization technique is used to calculate the transference of ion (T¬ion). The concentration and mobility of charge carries were calculated to explain the change in conductivity.

***Corrsponding Author: saxena.electronics@gmail.com**

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Invited Talk-17

Ionic and Spectroscopic Study of the Biocompatible Plasticized Polymeric Membrane for EC Device Application

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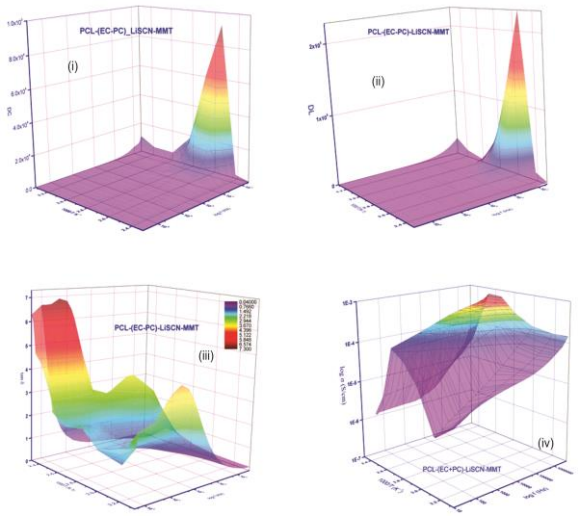
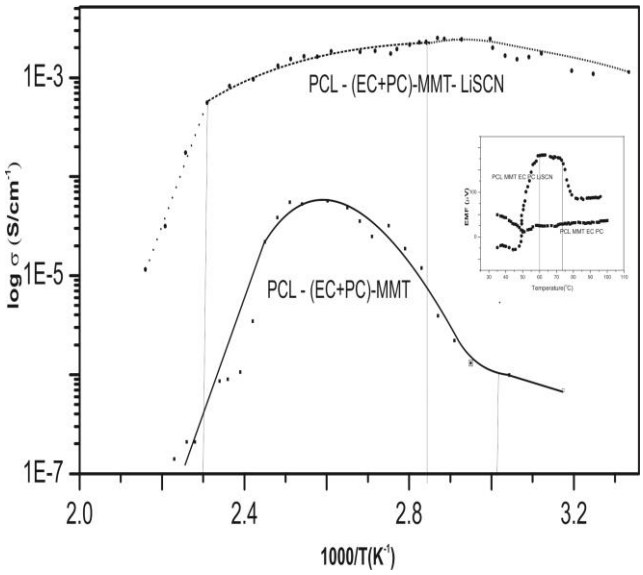
Abstract :

Biodegradable polymers received considerable attention due to their contribution in the reduction of environmental concerns. The incorporation of inorganic particulate fillers has been proved to be an effective way of improving the mechanical properties and in particular the toughness, of PCL (Polycaprolactone), MMT (Montmorillonite). Recently MMT become the most important clay filler due to their abundant presence in the nature. It possesses layered structure with an octahedral aluminum layer located between two layers of silicon tetrahedral. Each layered sheet is about 1nm thick with lateral dimensions of 100-1000 nm.



Variation of electrical conductivity, dielectric relaxation parameters with frequency and temperature



Conductivity of the PCL (EC+PC) MMT and PCL (EC+PC) MMT: LiSCN composite

This work described the development of a biodegradable polymeric composite electrolyte based on PCL, salt and MMT clay. The composite polymer film presents much better biomedical, thermal stability and anti-aging properties than the pure PCL polymer film. Environmental friendly lithium ion conducting $0.8\{[0.3PCL + 0.7(EC+PC)]_{40}: MMT_{60}\} + 0.2LiSCN$ complex polymer electrolyte films have been prepared through solution cast technique. Polymer nanocomposite electrolyte membranes were studied by XRD, FTIR with ATR spectrophotometer, Raman spectroscopy and Impedance analysis. Variation of dielectric functions with frequency and temperature shown in above figure. The dielectric constant and loss shows the low frequency dispersion behavior. The low frequency dispersion in the composite electrolyte is obtained due to interfacial polarization. The increase in voltage or the decrease in ionic conductivity is possible due to dissociation of the salt in electrolyte. After the addition of salt in the polymer – clay composite system enhanced the electrical conductivity up to 3-4 order The relative degree of crystallinity of PCL decreases as the LiSCN and plasticizers are added. The increase of ionic conductivity and dielectric constant is an indication of dissociated ions in the polymer matrix. The properties also discussed in the full manuscript. The synthesized electrolyte is used in different electrochemical devices like Fuel cell, Gas sensor as well as some medical applications.

Invited Talk-18

Determination of charge carrier concentration and mobility in polymer electrolytes: Space charge relaxation modelling approach

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Abstract

Polymer electrolytes are the key components for many applications in the field of electrochemical energy conversion and storage, for example, in batteries, super-capacitors, fuel cells and dye-sensitized solar cells. Evaluation of ion transport parameters is extremely important for the development of suitable electrolytes for specific application. However, despite numerous efforts, the mechanisms of ion transport are still not well understood. In the present work a new approach based on space charge relaxation modeling of impedance and dielectric spectroscopy data has been used to deduce the mobile charge carrier concentration and the mobility of ions in polymer electrolytes. Since the method is based on impedance analysis, it has advantages compared to potentiometric and amperometric electrochemical analysis techniques in that a small perturbation potential is applied across the electrolyte which minimizes the possible changes in charge carrier concentration during the measurements. The estimated values of mobility and charge carrier concentration for different polymer-salt systems appears to be much reliable in comparison to the other methods suggested in the literature.

Effect of polyaniline capping on the Optical Properties of ZnS/Mn Quantum Dot

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Keywords: Polyaniline (PANI); ZnS/Mn Quantum Dot; Optical properties

Abstract

In this work, we have presented synthesis of PANI capped ZnS/Mn quantum dot particles by chemical precipitation method, the structural and morphological properties of the composite material were investigated using X-ray diffraction (XRD) and transmission electron microscope (TEM). The average size of quantum dot were observed to be <5 nm which further decreases with increasing capping weight percentage. Fourier transform infrared (FTIR) spectra confirm the presence of vibrational modes of the ZnS with Mn and PANI ions in the samples. Photoluminescent (PL) and UV-Vis studies were carried out for optical properties of the uncapped and capped ZnS/Mn quantum dot. The UV–Vis spectra show the presence of red shift in the absorption peak along with an increase in band gap attributable to the quantum confinement effect. This red shift increases as the weight percentage of capping agent increases on ZnS nanoparticles. Photoluminescence (PL) emission spectra exhibit increased intensity in the visible region and UV region for the PANI capped ZnS/Mn samples. PL emission and other properties of these materials shall be selected as a suitable candidate for optical device applications.

Synthesis and Developement of Cellulose Based Alovera Nanocomposites Membrane for Food Packaging

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Abstract:

Polyvinyl alcohol (PVA) is a Non-toxic and water-soluble synthetic polymer. PVA used in production industry applications because of its biocompatibility, low toxicity and good adhesive properties. In present work, the bio-degradable composite films are prepared by waste product such as wheat-husk, coconut fibers. The wheat husk powder is prepared from alkali processes. It is low price, light-weight. Coconut fibers are eco-friendly, pollution free natural fibers. Aloe- vera consists of properties such as adhesive properties, flexural strength and good longitudinal tensile strength. The polyvinyl alcohol based composite films are prepared by solution -casting method. Synthesis improvement of Tensile strength testing, Thermogravemetric analysis (TGA).The composite films were subjected to mechanical properties such as tensile strength, %elongation, young modulus and surface properties. Structural behaviors are studied by Scanning electron microscope (SEM), Fourier transform infrared(FTIR)Spectroscopy and Differential Scanning Calorimeter (DSC).

Synthesis of polyvinyl alcohol (PVA)- Polyaniline (PANI) composite membrane for electrochemical devices

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Abstract

Polyvinyl alcohol (PVA) is a synthetic polymer having wide-spread applications in various fields. After membrane formation, it becomes very flexible. PVA itself does not show any conducting behaviour but very useful as a host polymer to hold others conducting salts or co-polymers. On the other hand, Polyanniline (PANI) is a semi-flexible conducting polymer. PANI, along with PVA in the polymeric membrane, shows conducting behaviour. Without the presence of any salt, this type of polymeric membrane shows good ionic conductivities. In present study, we have synthesized PVA-PANI membranes with their different compositions and characterized with Hioki impedance spectroscopy to measure their ionic conductivities. Also the synthesized membranes are characterized with infrared spectroscopy and X-ray diffraction spectroscopy. The PVA-PANI membrane is also able to sensing humidity in the ambient. Depending on the humidity of the ambient, the conductivity of the membrane also changes which is the subject of interest in the present study.

"Synthesis and Characterization of Rare Earth doped Y_2O_3Phosphor Material"

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Abstract

Scientists are working on phosphors since long time due to their wide applications in various fields. Rare earth metal-doped yttrium oxide has attracted much attention of scientific community due to its wide range of applications in display technologies. The phosphor has good luminescent characteristics, acceptable atmospheric stability, and low degradation under applied voltages, and no hazardous constituents as unlike to sulfide phosphors.

In particular, the nanostructured phosphor materials are of great interest as they offer brighter cathodoluminescence and much improved screen packing. Inorganic nanoparticles manifest unique size and shape (surface to volume ratio) dependent properties, which in some extent depend on their crystallinity, defect contents, and preparation techniques. In literature large number of reports are found on inner transition metal doped Y_2O_3:nanostructures in which different morphologies have been synthesized by using different methods such as gas phase condensation technique, sol-gel route, homogeneous precipitation, spray pyrolysis, and hydrothermal method by various research group.

In the Present work we have synthesized phosphor material using Y_2O_3 as host material and rare earth metals *viz.*, Gd, Tb as dopant. The synthesized phosphor materials have been analyzed by XRD and photo luminescence (PL). Using obtained data the effect of concentration of dopant on morphology and conversion efficiency/ luminescent property of phosphor materialhave been studied.

Effect of Rare earth element Doping on Structural and Magnetic Properties of Ni-Co mixed spinel Nanocrystalline Ferrites Synthesized by Sol-gel Auto Combustion Method

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Abstract:

Rare earth Neodymium (Nd^{3+}) doped nanocrystalline Ni-Co mixed spinel ferrites which are chemically represented as $Ni_{(1-x)}Co_xNd_yFe_{2-y}O_4$(x = 0.0, 0.2, 0.4, 0.6, 0.8, and 1.0 and y= 0.025 to 0.125, in the step of 0.025) were synthesized by sol-gel auto-combustion method. The structural, morphological, infrared and magnetic properties were studied in detail in the light of Nd^{3+} doping using standard techniques. X-ray analysis reveals the formation of single phase cubic spinel structure for all the prepared samples without any impurity phase. The crystallite size calculated from Scherrer's formula was observed to be decreasing with increasing Nd^{3+} content. The lattice parameter calculated using XRD data was found to be decreasing upto x= 0.100 and then increases for x = 0.125. X-ray density was observed to be increasing from 5.327 to 5.630 gm/cm^3. Surface morphology was studied through scanning electron microscopy technique. Grain size calculated from SEM analysis was found to be in the range of 30 – 59 nm. From transmission electron microscopy study, the average particle size was observed to be in the range of 35 - 45 nm. FTIR results exhibit the characteristics cubic spinel ferrite nature of the samples with two prominent absorption bands near 400 cm^{-1} and 600 cm^{-1}. FTIR also confirms the incorporation of Nd^{3+}in the crystal structure. The magnetic behavior shows strong influence of substitution of Nd^{3+}ions. The saturation magnetization, Coercivity and remenance magnetization all decrease with substitution of Nd^{3+} ions up to x = 0.100. For further increase in Nd^{3+} concentration (x = 0.125), the saturation magnetization found to be increased.

Keywords: Ni-Co Ferrites; Nd^{3+} doping; Sol-Gel Auto combustion; XRD, SEM-TEM, VSM.

Graphitic Carbon Nitride as Water Purifier: A Review

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Abstract:

Recently, water pollution has been a burning issue owing to hastily growing industrialisation and urbanisation. Phenolic derivatives as industrial raw materials or intermediates are quite indispensable in several industries like food additives, hair dyes, dyes, plastics, synthetic fibres, textile, paper, pulp, steel, petrochemical, petroleum refinery, rubber, dye, plastic, pharmaceutical, cosmetics, insecticides, weed killers, etc. However, excessive use of these causes environmental hazards and severe human health problems.

There are several methods and several materials that help the water to get free from such kinds of contaminations. The materials include several oxides like zinc oxide. copper oxide etc or carbon nanostructures like carbon nanotubes, graphene. Also few other materials like activated charcoal, zirconia can effectively remove such contaminants by different processes like adsorption, photo catalysis and many other.

Graphitic carbon nitride (GCN) is a special class of such triazine group consisting materials which exhibits two-dimensional sheet like morphology and very distinctive chemical, electronic and optical features arising from its highly delocalized π-conjugated polymeric framework. GCN in its pristine, doped and functionalized forms can be effectively utilised in numerous applications especially in water purification. There are many existing research works which have focused in details into the extensive adsorption and catalytic activities of GCN which have helped it to establish as a prosperous water-purifier nanomaterial.

This work will review the application of pure and doped GCN in the field of water purification and in connection the basic of different purification technology will also be discussed.

This detail discussion will surely help the researchers working in this fields to enrich their knowledge and thus to enhance the quality of their work.

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4.

Keyword: Water purification, Graphitic carbon nitride, adsorption, dye, catalysis

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Synthesis and Characterization of Graphene-Composite Foam

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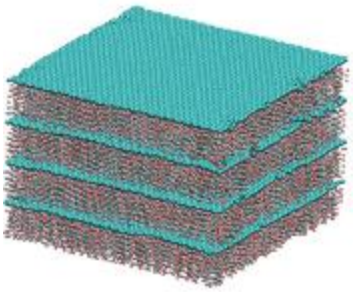
The superior mechanical properties of three-dimensional (3D) graphene foams have gained a great deal of attention from material scientists and energy engineers due to the combined benefits of both porous materials and two-dimensional (2D) graphene sheets. To research graphene reinforced composite foam's uniaxial super-compression and recovery behavior, we conducted comprehensive dynamics simulations of the material in ABAQUS. The foam simulations are produced by proliferating kelvin 3-D unit cell structure of graphene and composite material to form multilayered structure of material with graphene layers as basic structure of lattice with composite material layers in stacked between them.



Established periodic structures of graphene composite foam have the potential to achieve mechanical strength in terms of compression and regaining of the strength. The material is produced by a soft porous periodic lattice sample by polymerization of the emulsion continuous phase and by removing the solvent minority phase and then its predicted stress-strain values and young modulus are experimentally validated. In order to build soft periodic foam structures for the desired structural response and to monitor the effect of structural modes on acoustic response, the approach presented here will be useful. The study offers an effective way to understand 3D graphene composite foams mesoscopic physical existence and can, therefore leads to micro/meso/macro mechanical performance multiscale computational and optimal design of advance graphene foam-based material.

Keywords: Mesoscale, stress-strain curve, graphene composite foam, supercompression, recovery behavior

Scaling Exponents in 2+1 Dimension for Random-Ballistic Competitive Growth Model

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Abstract:

The interface width $W(L,t)$ of a rough surface evolves with time with two major variation type – dynamic growth with time is characterized by growth exponent β and saturation behaviour is characterized by roughness exponent α. Such different regions of surface evolution are separated by critical time. The overall evolution of the rough surface is best described by Family-Vicsek scaling ansatz as $W(L,t) \sim L^{\alpha} f(t/L^{z})$, where $z(=\alpha/\beta)$ is the dynamic exponent, $f(u) \sim u^{\beta}$ for $u \ll 1$ and $f(u) \sim constant$ for $u \gg 1$. The rough surface was developed through computer simulation for Competitive Growth between Random Deposition (RD) with probability $1-p$ and Ballistic Deposition (BD) with probability p in 2+1 dimension on a square plane $(L \times L)$ for system size L (16, 32, 64, 128 and 256) to record the statistical average of time variation of surface roughness $W(L,t)$ & average height $H(t)$ along with porosity σ for the model for different set of values of L and p. From this the scaling exponents were estimated. The growth appeared with two regions along with saturation with two acutely different slopes, β_1 and β_2 β_1 found to be independent of L but have some dependence on p. β_2 found to be independent of both L and p. The roughness for the saturation region found to have some dependence on p. The roughness exponent α found to be independent of p. The value $\alpha + \alpha/\beta_2$ found to be independent of both L and p. The first critical time t_{x1} found to be independent of L and have some exponential dependence on p. The second critical time t_{x2} found to have some dependence on both L and p. The fractional porosity found to be independent of L and have some exponential dependence on p. The scaling exponents found to have some deviation from the universality class and dependence on system size for the model.

***Keywords*: competitive growth model, random deposition, ballistic deposition, scaling exponents.**

Photo-switching Behaviour of Chemically synthesized Lead Sulphide multi armed Dendritic crystals

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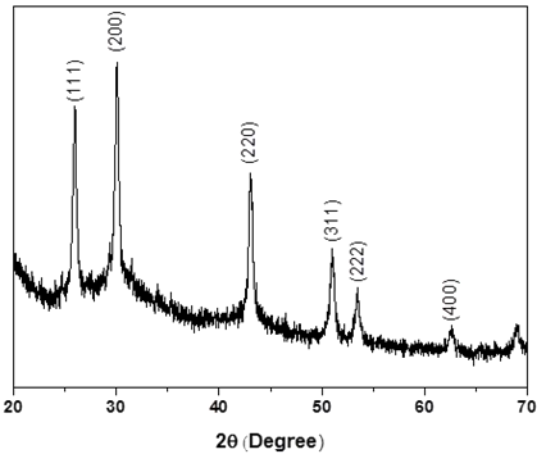
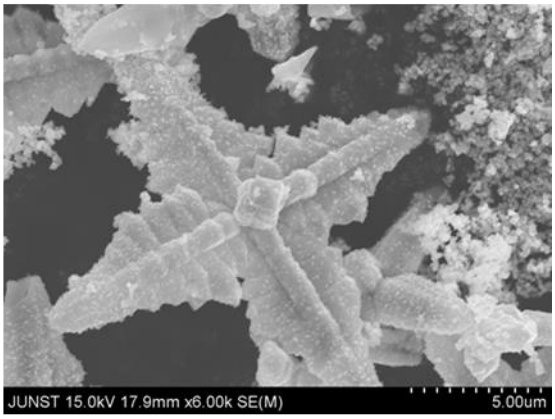
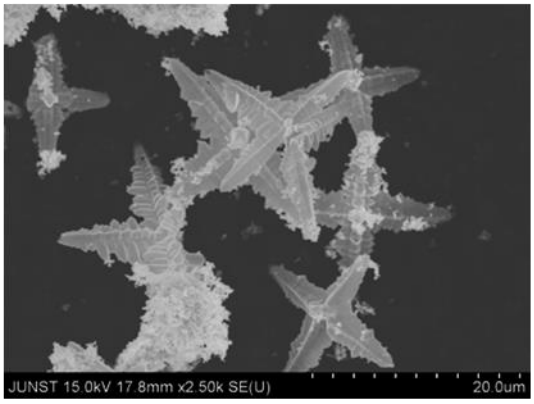
Abstract:

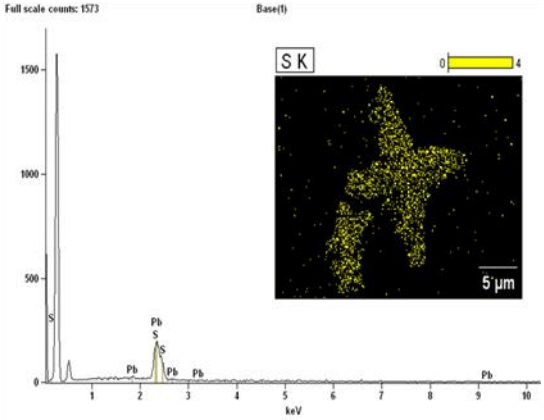
PbS is a member of the important and classical group IV-VI semiconductors. It is a widely studied semiconductor with a narrow energy band-gap (0.41 eV) and relatively large Bohr excitation radius (18 nm). Nanostructured PbS crystals show extensive quantum-confined effects and promising applications in optoelectronic devices such as light-emitting diodes, infrared detectors, infrared sensors, biological imaging, optical switches, solar cells,etc. Several methods have been used for the preparation of PbS nanocrystals including Sol–gel, Micelles, Langmuir–Blodgett Films and Solution phase method (chemical synthesis). Among them, the hydrothermal method provides a more promising way for the synthesis of crystals due to its low cost, high efficiency and potential for large-scale production.

Keeping all these in mind here we have reported the synthesis of multi armed PbS dendrites nanostructure by chemical bath deposition in powder form. The microstructures of the as synthesized materials were studied with the help of field emission scanning electron microscope. The successful phase formation was confirmedby X-ray diffraction which also shows that the material is of cubic crystal structures. The composition was analysed by energy dispersive X-ray analysis that shows a Pb/S ratio perfect for the proper phase formation. The as synthesised sample shows an efficient photo-response property with very short rising time and decay time suggesting the possible use of the material as optical switch.









Keyword: Lead sulphide, FESEM, XRD, EDX, Photo-conductivity

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Synthesis of highly conducting ionic liquid incorporated polymer electrolyte and porous carbon material for efficient supercapacitor

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Abstract

Herein, we have reported the highly porous carbon material synthesized from Poly(vinyl chloride) (PVC), activated by cobalt chloride ($COCl_2$). Additionally, the polymer electrolyte based on host matrix PVDF-HFP incorporated with ionic liquid 1-ethyl-3-methylimidazolium thiocyanate in an optimized ratio (20:80) was used as an electrolyte. Characterization for porous carbon like Energy-dispersive X-ray spectroscopy (EDX), X-ray diffraction, Brunauer-Emmett-Teller (BET), Scanning Electron Microscopy (SEM), Raman, Thermogravimetric Analysis (TGA) were carried out in detail. So, after synthesizing successfully the porous carbon we have fabricated an EDLC using polymer-electrolyte incorporated with ionic liquid and the specific capacitance calculated using cyclic voltammetry was approximately reaching to 300 F/g.

Keywords: Electric Double Layer Capacitor, Ionic liquid, Cyclic Voltammetry, Porous Carbon, Low Frequency Impedance Spectroscopy.

Recent development and challenges in Zinc oxide (ZnO) based Gas Sensors

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Abstract

Zinc oxide is a non-transition metal oxide compound semiconductor and one of the transparent conducting oxide (TCO) and promising material for semiconductor device applications. The gas sensor is simply an artificial nose, which can smack odourless gas along with any smell. Gas sensor is one of the devices, which is used to identify the presence of respective gas and is used for both quantitative and qualitative purposes. For the purpose of gas sensing material ZnO based structure have been developed. In this study, a systematic report has been presented. Different metals were used as doping element and various nanocomposites have been prepared with ZnO. Mostly used doping elements were Au, In, Ag, Al, Pd, Cu and the nanocomposites were prepared like CuO-ZnO, PdO-ZnO, TiO2-ZnO, SnO2-ZnO, NiO-ZnO, Fe2O3-ZnO, CdO-ZnO, Cr2O3-ZnO and MnO2-ZnO. After reviewing these result the changes in this technology have been presented.

Geometry optimization vibrational frequencies electronic properties of Urecil Mustred by using DFT

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Abstract

The geometry optimization of Urecil Mustred has been done with combination of DFT/B3LYP method and 6-311G (d, p)/6-311++G(d, p) basis set. The correlation factor (R^2=0.987) for 6-311G (d, p) and (R^2=0.995) for 6-311++G(d,p) shows that calculated vibrational frequencies of Urecil Mustred is well matched with experimental IR frequencies.The electronic properties of title molecule are calculated with help of HOMO,LUMO,MESP plot.The calculated energy gap(4.02eV) of title molecule shows that title molecule is chemically reactive. Several electronic and thermodynamical parameters are also calculated with same level theory. The Calculated hyperpolarisibilty of title molecule shows title molcule is good NLO activite agent.

Kay Word: Urecil Mustred**, DFT,** NLO

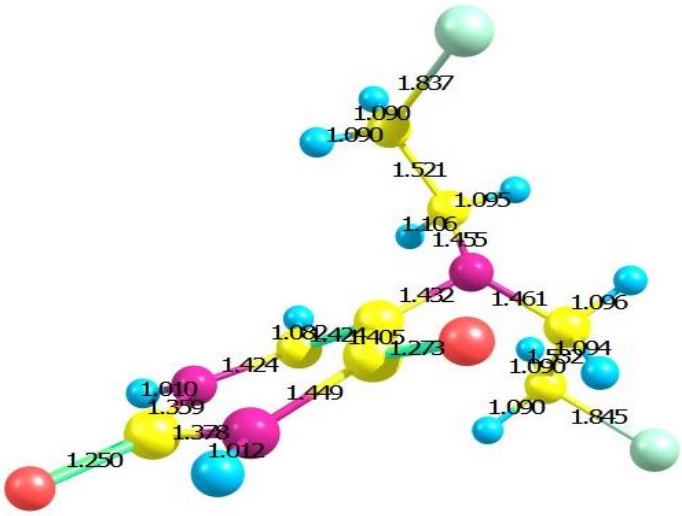

Fig-1 Optimized Geometry of Urecil Mustred

DFT study of superhalogen properties YCl_n (n=1-6) complexes

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Abstract

In present communication a systemic study on YCl_n (n=1-6) have been studied by using combination of DFT/B3LYP method and SDD basis set. The six Cl atoms are bound to a single Y atom. The Superhalogen behavior of YCl_n complexes successively increases as number of Cl atom increases and reaching a peak value of 8.4 eV for YCl_6. The calculated dissociation energy of YCln complexes through Cl_2 channel shows that all species are stable against dissociation through Cl_2 channel. This curious binding character of Y atom with different Cl atom are explained by involvement of inner shell d electrons, which not only allow YCl_n complexes belong to the class of superhalogens. Some electronic parameters of YCl_n are also calculated by using same level theory.

Keywords: Density functional theory; Superhalogen

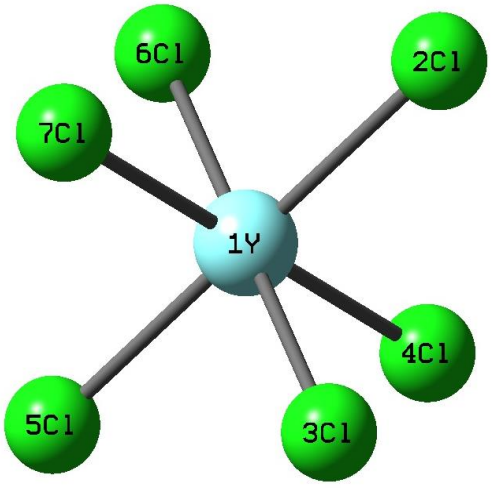

Fig-1 Optimized geometry of Anion of YCl_6

DFT Study of Structural, Electronic and magnetic properties of Half-metallic Full-Heusler Alloy Ru_2VSb

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Abstract:

Half-metallic ferromagnetic (HMF) materials have attracted much attention over the years because of their application in Spintronics based devices, as they show spin -polarization at Fermi-level. In the present paper, structural, electronic and magnetic properties of ruthenium based full – Heusler alloy Ru_2VSb have been studied using first-principles calculations based on Khon-Sham Density Functional Theory (KS-DFT). Pseudo-Potential Plane Wave method within Generalized Gradient Approximation (GGA) was employed for the present calculations. Density of states and band structure calculations show that the present alloy is half-metallic in nature with 100% spin-polarization at the Fermi-level. The equilibrium lattice parameter and bulk modulus were also computed by fitting the total energy versus volume of the unit cell to the Murnaghan's Equation of State. The calculated total magnetic moment per formula unit is also consistent with the Slater-Pauling Rule for Half-Metals.

Index Terms: DFT, Pseudopotential-method, Half-metallicity.

High Conducting PVDF-HFP+PTA polymer electrolyte for Supercapacitor application

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Abstract

Herein, we reported the synthesis of polymer electrolyte prepared using polymer PVDF-HFP and PTA doped using well known solution cast technique method. There was a huge hike in the conductivity recorded while incorporating of PTA with polymer PVDF-HFP which was scrutinized by complex impedance spectroscopy. Fourier transform infrared spectroscopy was done to check the complexity of blended polymer PVDF-HFP with PTA. Polarized optical microscopy was also done to check the amorphousity of the polymer electrolyte. A good stable Electric double layer capacitor was fabricated using optimized polymer electrolyte film which shows reasonable efficiency.

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Enhanced Photoluminescence properties of Na^{+} co-doped $SrAl^{2}O^{4}$: Eu^{3+} chain like nanophosphor for solid state lighting application

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Abstract

In recent days, rare-earth doped phosphors have attracted an immense attraction in luminescence field for solid-state lighting and display device applications[1, 2]. However, need of efficient red light emitting nanophosphor is still a major challenge for fabrication of such devices. Herein, we report a bright red light emitting Na^{+} codoped $SrAl_2O_4:Eu^{3+}$ chain like nanophosphor which is synthesized by modified sol-gel technique. These nanophosphors show excellent red emission due to $^5D_0 \rightarrow {}^7F_j$ (j = 1, 2, 3, 4) transitions of Eu^{3+} ions excited by 394 nm [2]. Photoluminescence studies of both Eu^{3+} doped $SrAl_2O_4$ and Na^{+} - codoped $SrAl_2O_4:Eu^{3+}$ has shown more than two fold increases in intensity on optimum Na^{+} addition. The improved lifetime obtained from decay study has shown that the co-doped Na^{+} has successfully reduced the non-radiative transitions. The results suggest that this efficient nanophosphor could be a major candidate in the growing field of solid state lighting applications.

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Improved photocatalytic activity of Zinc Cadmium Sulfide under Visible Light Irradiation

Ankita Chandra[a, 1], Shrabani Ghosh[a,1], Samrat Sarkar[a], Nirmalya Sankar Das[b,c], Madhupriya Samanta[a], Sourav Sarkar[a], K.K.Chattopadhyay[a,b*]

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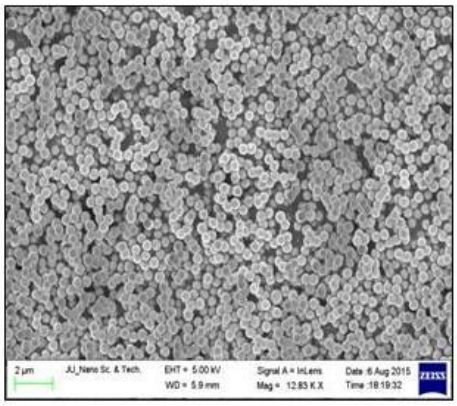
ABSTRACT

Development of textile dyeing industry leading to environmental problems related to toxic organic pollutants initiates the research of environmental management through photocatalytic treatment efficiently. Besides, unusual depletion of conventional fossil fuels in high rate and environmental hazards associated with the use of this carbon-emitting fuels have attracted the researcher to find an abundant, everlasting, zero-emitting and eco-friendly combined fuel source as an alternative.[1] Hydrogen can be considered as highly efficient, low polluting fuel and it can be utilized for transportation, heating and power generation in some places where utilization of electricity becomes difficult. Here, $Zn_{0.8}Cd_{0.2}S$ microspheres are synthesized which act as a very efficient photocatalyst for MO dye degradation and H_2 evolution in presence of visible. To study the relevant properties of the material, different characterizations like XRD, UV-VIS, FESEM are performed. XRD peak determines the formation of solid solution by peak shifting and zinc blende phase of obtained material. FESEM shows formation of uniform micro-spherical structure with diameter of nearly 430 nm. UV-Vis spectroscopy gives the bangap value of 2.83 eV. Under visible light spectra, it helps to degrade 86.2 % of MO dye within 105 minutes with a reaction rate of 1.71×10^{-2} min^{-1} and 15.66×10^{-2} min^{-1} using Pseudo 1st Order Reaction Kinetics and Modified Freundlich Model respectively. The hydrogen production reaction is performed via hydrolysis of $NaBH_4$ and the generation of hydrogen rate is increased in presence of $Zn_{0.8}Cd_{0.2}S$ in presence of visible light lamp with TOF 88.28 ml gm^{-1} min^{-1}. It can be concluded that preferred bandgap, sufficiently negative conduction band edge and uniform structural property can be key factors for such an impressive catalytic activity which is better than ZnS or CdS.



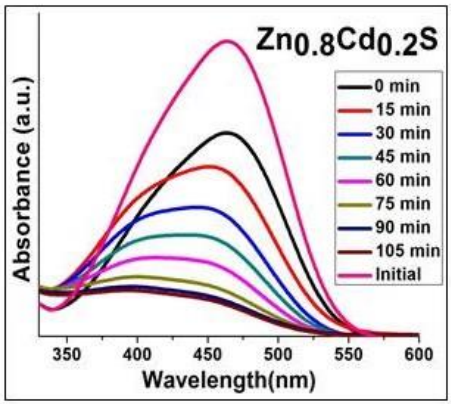


Figure 2: MO degradation (under visible)

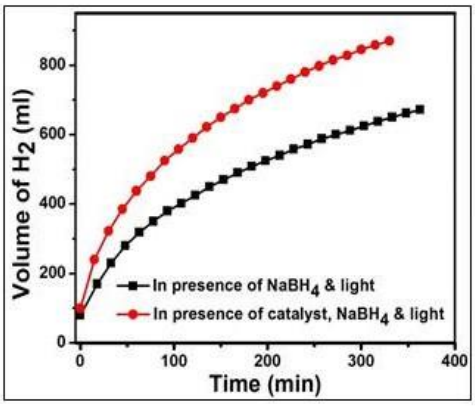


Figure 3: H_2 production

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Optical properties of Al-doped ZnO Thin Film deposited by Sol–Gel route

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Abstract:

Transparent conducting Al-doped Zinc Oxide (ZnO) thin films were successfully deposited on glass substrates by sol-gel spin coating technique. The XRD, UV-visible spectroscopy, Raman spectroscopy and fluorescence spectroscopy were utilized to study the structural, optical, vibrational and fluorescence properties of the thin film. XRD shows that deposited thin films has hexagonal wurtzite structure with preferential orientation along c-axis. The UV-visible transmission spectra reveals that the deposited thin films have the transmittance greater than 80% in the visible region which indicates that ZnO thin films can be utilized as transparent conducting oxide (TCO). The value of band gap calculated from the Tauc's plot has been found to be ~3.28eV, which is less than that of the bulk ZnO material i.e. ~3.37 eV. The fluorescence spectrum showed a emission peak at about 397nm, originated from the exciton recombination corresponding to the near band edge transition (NBE) of ZnO. The visible emission peak at about 527 nm corresponds to the green emission which is attributed to the oxygen vacancies and antisite oxygen.

Keywords: ZnO thin films, sol-gel, Fluorescence spectroscopy, Energy Band gap

Realization of theoretically predicted cold electron emission from oxide perovskite: vanadium doped $BaSnO_3$ nanocubes

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Abstract

In search of an efficient cold cathode out of the perovskite systems, vanadium doped $BaSnO_3$ nanocubes were synthesized via traditional solid-state reaction method. Thorough characterization via X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM) and energy dispersive X-ray (EDX) studies showed the proper phase formation, grain related information and composition related investigation. To avoid repetitive experimental attempts and to optimize cold electron emission capability of the doped and undoped system, ANSYS-MAXWELL simulations for field emission properties was carried out. The dielectric constant, bulk conductivity, dimension of the nanocubes and virtual conditions identical to actual cold cathodes were used as input parameters for the simulation procedure to achieve maximum possible realistic predictions. Emboldened by positive theoretical outcome, actual field emission experiments were carried out under a high vacuum chamber. The emission current density of $BaSnO_3$ doped with 5% vanadium showed a maximum of 0.5 mA/ cm^2. The turn on field was reduced by 30% for 5% vanadium doped sample compared to the pristine one. This work opens up a new field for $BaSnO_3$ based perovskite system beyond capacitor in display and other devices.

Keywords: ANSYS-MAXWELL, $BaSnO_3$, perovskite, pristine.

Morphology modulated Ga_2O_3 nanostructures for green water purification technology

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Abstract

In recent years, various fabrication methods of photocatalytic materials have been developed for photo degradation of organic and inorganic pollutants from consumable water. Particularly, inorganic semiconductor nanomaterials have been considered as most promising agents for photocatalytic applications due to their remarkable physical and chemical properties with large effective surface area, and a variety of morphologies, such as nanorods, cubes, spheres and flowers, synthesized by cost effective chemical route. This work is directed towards the development of group III metal oxide nanostructures of Ga_2O_3 which have been recognized as an important material for several applications including catalysts, gas sensors, solar cells, photodetectors etc. Typically, the Ga_2O_3 nanostructures were obtained by calcination of gallium oxide hydroxide synthesized via a chemical bath method. Then, as-prepared hydroxide nanostructures were calcined at 800° C for 3 hours for obtaining Ga_2O_3 nanostructures. This system was characterized by traditional tools like XRD, FESEM, HRTEM, EDX, UV-Vis to investigate the phase information, morphological features, composition and the information about band gap of the same. Also, the photocatalytic performance of as-prepared and commercially available Ga_2O_3 nanostructures were studied by time evolved UV-Vis absorption spectrum of degradation of different types of organic pollutants like Rhodamine B, Methyl Orange and Eosin B solution. Under UV irradiation, the as-synthesized Ga_2O_3 nanostructures exhibited a high photodegradation efficiency which is a remarkable enhancement over the identical performance of commercially available one. This work proposes a simple cost effective eco-friendly route for synthesis of Ga based oxide photocatalysts for wastewater treatment.

Keywords: Gallium oxide; Photocatalytic performance; nanostructures; Dye degradation

Doped g-C_3N_4 : an Efficient Water Purifier

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Abstract

Textile industries have been one of the oldest and essential industrial sectors making it one of the major contributors in the economic growth of any country. India has been one of the major contributors in this field. However, due to ever increasing demand of textiles, the industries are forced to use more dyes to make its produce. And the effluents from the textile industries are often not filtered properly posing an environmental threat. Rhodamine B is a known carcinogenic element which is often used in textile industries for its characteristic red colour.

The work describes the synthesis of a europium (Eu) doped graphitic carbon nitride using solid state synthesis route using two primary precursors. The proper phase formations were confirmed for both the materials, pure and doped, by x-ray diffraction. The SEM micrographs exhibits the microstructure of the samples and the successful doping were confirmed by the energy x-ray dispersive analysis. The optical properties were investigated by UV-visible spectroscopy and the Fourier transformed infrared spectroscopy confirmed the presence of expected chemical bonds. The effect of doping on the photoluminescence (PL) property of the samples were studied using a photoluminescence (PL) spectrophotometer. The samples show excellent photocatalytic activity in the removal of textile dye like Rhodamine B under UV irradiation. The photocatalytic efficiency increases with the increase in doping concentration up to a certain limit. A probable mechanism behind the photocatalytic activity in the removal of Rhodamine B from the water is also given.

Keyword: Graphitic carbon nitride; Europium; Photoluminescence, Photocatalysis, Rhodamine B, Water purification

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Thermodynamical study of Oxide glass forming melts

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Abstract

The study of thermodynamic behavior of oxide melts have been studied with the help of thermodynamic parameters. The most important parameter Gibbs free energy difference (ΔG) can be calculated with the help of experimental values of specific heat difference between under cooled melt and equilibrium solid phases, but due to the strong tendency of crystallization, it is very difficult to measure the thermodynamical parameters experimentally, consequence, theoretical estimation of these parameters becomes highly beneficial. In the present study, the thermodynamic behaviour of glass forming melts for three samples of oxide glass forming melts B_2O_3, GeO_2 and SiO_2 in the entire temperature range T_m to T_g using the expression obtained based on the hole theory of liquids.

Key words: Oxide melts, Gibbs free energy, thermodynamics of undercooled melts.

O-23

Fabrication of bismuth ferrite multiferroic lead-free high T_C ferroelectric material

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Abstract

The Mn-doped $BiFe_{1-x}Mn_xO_3$ (x=0.00 to 0.10) nanomaterials have been prepared by co-precipitation method. The powder x-ray diffraction pattern analysis shows a structural phase transformation from rhombohedral to orthorhombic, as Mn content increases from x=0.00 to 0.10. The Raman spectrum analysis also confirms structural phase transformation. The average crystallite size was calculated using Scherer formula and found to decrease from 100 to 80 nm. The surface structure of interconnecting cubic grain turns into spherical grains via petal shaped grains with increasing the Mn-doping concentration. The value of dielectric constant at the frequency of 1 MHz increases rapidly from 27.2 to 76.8 where as the tangent loss (Tan δ) increases gradually from 0.26 to 0.55 as the Mn-doping concentration increases from x=0.00 to 0.10. It reveals the enhancement of ferroelectric behaviour and suppression of the leakage current density. The drastic change in the phase image contrast of magnetic force micrographs with increasing Mn-doping concentration also indicates the improvement of the ferromagnetism.

Keywords: XRD; Surface modifications; Multiferroic.

COMPARISON OF EUGENOL AND PAPAIN - A REVIEW

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ABSTRACT

Eugenol is a compound found in certain plants, such as basil, cinnamon, lemon balm, and nutmeg, but is primarily extracted from clove plants. Papain is an endolytic plant cysteine protease enzyme which is isolated from papaya (Carica papaya L.) latex. Eugenol more effective uses in medical than papain. Papain helps explain how the proteolytic enzyme works and also makes it valuable for a variety of purposes. Eugenol is used as flavor, irritant, sensitizer and can produce local anaesthesia. Several bacterial infections are associated with the risk of certain cancer, and viruses are now recognized as the second most important cause of human cancer.

Keywords:, Anesthetics, Papain, Structure, Cancer, Eugenol, Proteolytic

Tuning transport properties of $CuBO_2$ via sulphur doping

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Abstract

$CuBO_2$ is a novel material in the research field of transparent conducting oxide. Mixing of different orbitals to achieve proper control on transport properties via shallow acceptor levels is extremely important in order to have an actual p-type transparent oxide involving delafossite. However, there are few attempts towards these. This study demonstrates an effective way out to achieve significant delocalization of holes in the (Cu 3d + O 2p) valence band with a direct gap by different chalcogen (Ch = S, Se) doping. A modulated valence band in $CuBO_2$ was achieved via sulfur incorporation at the O site. As a result, better transport properties were reflected in the doped material. Dispersion of Cu 3d character by incorporating shallower acceptor (Ch 3p) states is concluded upon analysing the photoemission spectra of the valence band. In this study we have synthesized $CuBO_2$ and sulfur doped $CuBO_2$ nanostructures via easy molten-salt method. Structural characterization was performed using X-ray diffraction (XRD) which confirmed good crystalline structure and proper phase formation. Field emission scanning electron microscopy (FESEM) revealed morphological information of the samples. The transport properties of the samples were studied using a "SMU" in room temperature. Here we discussed further how the conductivity of sulfur-doped $CuBO_2$ is increased up to a certain percentage of sulfur doping in $CuBO_2$, after that it will be decreasing.

PVDF-HFP + NaSCN and Ionic liquid based polymer electrolyte for supercapacitor

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Abstract

Based on poly (vinylidene fluoride-co-hexafluoropropylene) P(VDF–HFP) and sodium thiocyanate (NaSCN), solid polymer electrolyte (SPEs) films are prepared using the solution casting technique. Ionic liquid (IL; 1−ethyl-3-methyl−imidazolium tricyanomethanide ([EMIM][TCM]) is incorporated into the prepared polymer-salt complex matrix to further enhance its ionic conductivity. Polarized optical microscopy (POM) shows a change in the surface morphology of IL doped polymer electrolyte films. The composite nature of polymer electrolyte films is confirmed using Fourier transform infrared (FT−IR) spectroscopy via studying ion-ion and ion-polymer interactions. The structural morphology of ionic liquid doped polymer electrolyte films (ILDPE) confirms the complexation between the ionic liquid ([EMIM][TCM]), salt (NaSCN) and polymer P(VDF–HFP). This is further confirmed using DSC and XRD measurements. The XRD structural analysis confirms the intensity of crystalline peaks presents in IL doped solid polymer electrolyte films decreases compared to that of pure polymer as well as polymer salt complex system. XRD clearly indicates the enhancement in its amorphous nature which is necessary to increase the conductivity. The incorporation of IL into polymer salt–complex matrix leads to changes in melting of polymer electrolytes, confirmed by DSC thermograms. Polymer electrolyte films are also characterized using impedance spectroscopy (IS) to check their electrical properties. The highest ionic conductivity is found to be 7.80×10^{-4} S cm^{-1} for 6 wt% IL doped polymer electrolyte film. The Linear sweep voltammetry (LSV) analysis shows that the optimized polymer gel electrolyte is electrochemically stable up to 1.5 V. The ionic transference number (t_{ion}) is calculated and found to be 0.985. Electrical double layer capacitor (EDLC) has been fabricated using this highly conducting polymer electrolyte film and specific capacitance value is found to be 1.31 F g^{-1}.

Keywords: polymer electrolyte; electrical double layer capacitor; ionic transference number (t_{ion}); charge carriers; mobility; ionic conductivity.

A REVIEW ON THERMODYNAMIC ASPECTS OF BULK METALLIC GLASSES AND THEIR APPLICATIONS

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ABSTRACT

The bulk metallic glasses (BMGs) are a class of important engineering materials. BMGs have achieved a great interest of the investigators due to their superior physical and chemical properties. The formation of BMGs in multi-component metallic alloys has also prompted new interest for the understanding of non-crystalline materials due to their promising technological applications. The thermodynamic aspects of BMGS have been studied by calculating the Gibbs free energy difference (ΔG), entropy difference (ΔS) and enthalpy difference (ΔH) between the undercooled melts and corresponding equilibrium solid phases. Recent advances in the applications of BMGs have also been reviewed in the present study.

Keywords: Bulk Metallic Glasses, Thermodynamics, Gibbs free energy, Enthalpy, Entropy.

O-28

Study on Irradiated and Hydrogenated metal-Semiconductor Devices

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ABSTRACT

The current-voltage (I-V) characteristic is a fundamental characterization unit to measure the ideality of a junction device. The ideality of the device is a parameter to check the goodness of a device as for the requirement. The carrier transport mechanism of a junction device through interface can be well understood with I-V characteristics. The metal-semiconductor interface can be well studies with C-V Characterization tool. In the present study the I-V and C-V techniques are used to study the bulk as well as interface properties of metal semiconductor junction devices. The fabricated devices were characterized under three stages such as before irradiation, after irradiation and after hydrogenation of irradiated devices. The irradiations were done at IUAC, New Delhi with high energy heavy ions of different fluences. The results were discussed in terms of defects passivation of irradiated devices.

Key Words : Irradiation, M-S Junction, Hydrogenation, Fluences, Ideality Factor.

O-29

Third harmonic radiation generation by propagation of laser beams in under dense plasma

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ABSTRACT

Interaction of laser pulses with plasma is relevant to many nonlinear phenomenon including laser fusio[1], charged particle accelerators[2], and harmonic radiation sources[3]. The excitation of coherent radiation at harmonics of the fundamental frequency of the laser is of much practical importance due to its potential for producing x-ray lasers and coherent radiation sources[4]. Interaction of intense laser pulses with homogeneous plasma leads to the generation of odd harmonics of the laser frequency[5]. Even harmonics of the laser frequency can be generated by interaction of linearly polarized laser pulses with inhomogeneous plasma and also in the presence of external fields.

The present study deals with the phase-matched third harmonic radiation generation via laser plasma interaction. When an intense laser beam interacts with homogeneous plasma in presence of a transverse, static electric field, a transverse current density oscillating at the third harmonic frequency of the laser pulse is setup.

This leads to the generation of third harmonic radiation. The periodicity of the applied static electric field allows the harmonic radiation to be phase-matched

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Biological AIM analysis Fukuai Function caculation of Urecil Mustred by First Pincipal

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Abstract

Nitrogen mustards are basically have a fine useful class of anti cancerous drugs may used in several type of cancers. In present communication geometry optimization of Urecil Mustred has been done with combination of DFT/B3LYP method and 6-311++G(d, p) basis set. The AIM analysis shows that a weak electrovalent interaction occurs in between O_3-H_{17} with interaction energy is 3.150 kcal/mol. PASS analysis shows that title molecule shows good activity against Antineoplastic, Antiviral etc. The calculated full fitness score (--1192.23kcal/mol) and binding affinity (ΔG=-6.28kcal/mol) shows that Urecil Mustred well dock with 6LU7 protein which propose that Urecil Mustred have good potential for treatment of COVID-19.

Kay Word: Keyword: Density Functional Theory (DFT), 6LU7,COVID19

An investigation Superacidic properties of hydrogenated FeF_n^-(n=1-6): A DFT study

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Abstract

In present communication we suggest a new series of superacids by protonation of FeF_n^-(n=1-6) by using combination of DFT/B3LYP method and SDD basis set. From this study we conclude that acidity of superacids are connected to electronic stability of FeF_n^- . The calculated vertical detachment energy (VDE) shows thatFeF_n^- are belongs to superhalogenic family. The HOMO LUMO plots NMA dissociation energy of HFeFn shows that all species are thermodynamically stable. The calculated deprotonation energy of $HFeF_n$ suggest that all species for n>3 are belongs to family of superacids. The calculated deprotonation energy for n=6 specie are more acidic than $HSbF_6$ superacid.

Key words: Superhalogen, Superacid, DFT, Electronic properties, VDE

DFT study of Bioactive Agent - Proflavine

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Abstract

Proflavine, is antiseptic and anticancer drugs. The optimized geometry of Proflavine have been calculated by combination of DFT/B3LYP method and 6–311G (d, p) basis set. The correlation factor (R^2=0.99) suggest that calculated IR frequencies are well matched with experimental. The HOMO-LUMO analysis shows chemical reactivity of Proflavine. Nonlinear optical (NLO) analysis of the molecule is calculated with help of polarizibilty, first hyperpolarizability parameters. The several thermodynamic parameters of title molecule are calculated with same level theory. The calculated FF suggest that C_4 is most electrophilic and C_5 is most nucleophile charge center.

Keywords: DFT, T HOMO-LUMO, NLO

Synthesis of polyvinyl alcohol (PVA) capped ZnS nanosize particles: structural and morphological properties

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Keywords: Polyvinyl alcohol (PVA); ZnS Nanoparticles ; Photoluminscence

Abstract

In this work, we have presented synthesis of PVA capped ZnS nanosized particles by chemical precipitation method, the structural and morphological properties of the composite material were investigated using X-ray diffraction (XRD) and transmission electron microscope (TEM). The average size of nanoparticles were observed to be <5 nm which further decreases with increasing capping weight percentage. Photoluminescent (PL) and UV-Vis studies were carried out for photophysical properties of the uncapped and capped ZnS nanoparticles. The UV–Vis spectra show the presence of red shift in the absorption peak along with an increase in band gap attributable to the quantum confinement effect. This red shift increases as the weight percentage of capping agent increases on ZnS nanoparticles. Photoluminescence (PL) emission spectra exhibit increased intensity in the visible region and UV region for the PVA capped ZnS samples .PL emission, and another properties of these materials shall be selected as a suitable candidate for optical device applications.

HARTREE FOCK ELECTRONIC STRUCTURE STUDIES OF RITALIN AND CAFFEINE.

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ABSTRACT

Atomic charges, dipole moment and total energy of Caffeine and Ritalin were compared in order to explore the finer details of these molecules. HF/6-311G calculations have been performed on the electronic structure of Caffeine and Ritalin. Comparison shows that redistribution of charges on Caffeine is over larger range (- 1.053e to 1.053e) as compared to Ritalin from this we concluded that caffeine is more reactive as compared to Ritalin as it offer more reactive sites and having more energy as compared to Ritalin, further the same is also confirmed by our ADMP computation HF/6-311G. From this study it is very clear that why Ritalin is more euphoric in preference to caffeine and is farm more stimulating than caffeine.

Keywords:, Caffeine, Ritalin, Electronic structure, Net atomic charges, Bond length, Dipole moment.

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Low Frequency Electrical Behaiver of a fluorinated liquid crystalline material with phases

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Abstract

Electrical response of a fluorinated liquid crystalline material 7F6Bi have been investigated. Material exhibits paraelectric SmA*, ferroelectric SmC* and a wide temperature range (~ 83 °C) antiferroelectric SmC*$_a$ phases. The dielectric studies have been carried out in the frequency range of 1 Hz to 35 MHz under planar anchoring conditions of the molecules. The soft mode relaxation due to the tilt fluctuation of molecules in the MHz region has appeared in the SmA* phase, whose relaxation frequencies decrease with decrease in the temperature. Its dielectric strength increases (~ 0.2-3.4) with decrease in temperature and follows Curie-Weiss law. The Goldstone mode relaxation due to phase fluctuation of molecules with relaxation frequency ~ 10 kHz appears in SmC* phase. The dielectric response of the SmC*$_a$ phase exhibits unusually one relaxation mode due to anti ferroelectric ordering of the molecules. Its dielectric strength varies from ~ 0.55 at 104.3 °C to 2.20 at 37.6 °C. Switching parameters viz. spontaneous polarization, switching time and rotational viscosity have also been determined.

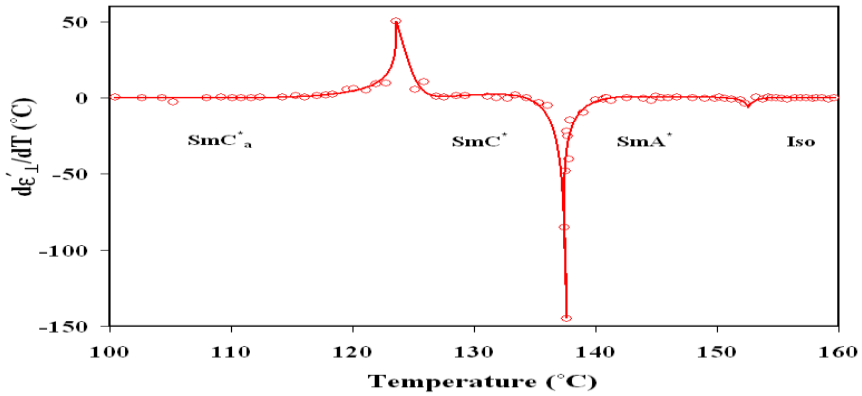

Figure 1 Temperature dependence of the $d\varepsilon'_{\perp}/dT$ at 100 Hz. Lowest value of the $d\varepsilon'_{\perp}/dT$ in the ferroelectric SmC* phase clearly distinguishes paraelectric SmA* phase (right) with the antiferroelectric SmC*$_a$ phase (left).

Microstructural Influenced Conduction Mechanism of Mn-doped Garnet type Solid Ionic Conductor

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Abstract

Garnet type solid-state electrolyte are receiving commendable attention owing to high safety, high ionic conductivity, negligible electronic conductivity, large potential window and high mechanical strength. Hence, they are very promising for developing all solid-state batteries. Though, the ionic conductivity of the garnet based $Li_7La_3Zr_3O_{12}$ (LLZO) system depends on its structural symmetry (cubic and tetragonal) and densification of the system. Another way to increase the conductivity is tune the Li content into the system with the optimized distribution of Li-ions in the octahedral and tetrahedral sites. In this regard, by multielement doping at different cationic sites high conductivity can be achieved. Further, doping of multivalent atoms on Zr sites can affect the Li occupancy and Li vacancy in LLZO framework, which plays a very crucial role for ion migration. Seeing the importance of dopant in conduction of LLZO, effect of Mn-doping for Zr in the garnet-type $Li_{6.25+y}Al_{0.25}La_3Zr_{2-y}Mn_yO_{12}$ (y = 0, 0.05, 0.1, 0.2) on ionic conductivity was investigated using electrochemical ac impedance spectroscopy. By doping of Mn on Zr sites, a correlation between the structural parameter, microstructure and the Li^+ ion conduction phenomenon is stablished in this study. Among all the investigated compounds, $Li_{6.35}Al_{0.25}La_3Zr_{1.9}Mn_{0.1}O_{12}$ exhibits highest total ionic conductivity of 3.5×10^{-4} S/cm at room temperature. The microstructural dependent Li-ion transportation and relaxation process during the conduction mechanism are discussed.

Reference:

1. Morphological, dielectric and transport properties of garnet-type $Li_{6.25+y}Al_{0.25}La_3Zr_{2-y}Mn_yO_{12}$ (y = 0, 0.05, 0.1, and 0.2), Brahma Prakash Dubey, Asit Sahoo, Venkataraman Thangadurai, Yogesh Sharma, Solid State Ionics, 351 (2020), 115339

Study of Stability and Protonic Conductivity of Composites Electrolytes (1-x)CsH_2PO_4 /xZrO_2 For Fuel Cells

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Abstract

Composites proton conducting material based on cesium dihydrogen phosphate were prepared and doped with zirconium oxide. We observed the Stability and Protonic Conductivity of composites proton electrolytes in terms of X-ray diffraction(XRD) analysis, Fourier Transform Infrared Spectroscopy(FTIR), Differential Scanning Calorimetry (DSC), Raman spectroscopy, and conductivity measurements. We have investigated that the ionic conductivity of undoped CsH_2PO_4 increases up to three orders of magnitude within the transition temperature 230^{o}C to 250^{o}C. We doped ZrO_2 with different composition (1-x) CsH_2PO_4/xZrO_2($0 \leq x \leq 0.4$). CsH_2PO_4 transition temperature from monoclinic to cubic phase is found at 230^{o}C. The stability, ionic conductivity, and fuel cell performance were investigated within the temperature range 230^{o}C to 280^{o}C under environments atmospheric humidification. The electrode on pellets was made by the vapor deposition technique of silver wire.

Keywords: composite, conductivity, cesium dihydrogen phosphate, Fuel, XRD.

Electrical Conductivity and Thermal Analysis of CsH_2PO_4(CDP)/NaH_2PO_4(SDP)/ZrO_2 Composites Electrolyte for Fuel Cell

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Abstract

Solid acid composite CsH_2PO_4(CDP)/NaH_2PO_4(SDP)/ZrO_2 were synthesized and characterized by a different molar ratio of CDP, SDP, and ZrO_2. The characterizations of the Solid acid composite were observed the thermal stability and conductivity in terms of X-ray diffraction (XRD) analysis, Fourier Transform Infrared Spectroscopy (FTIR), Differential Scanning Calorimetry (DSC), and conductivity measurements. The amount of CDP, SDP, and ZrO_2 pressure used for pallet production and operating temperature. The composites powders were to form pellets of 3 mm thickness for conductivity measurement. SDP in the composites has a large effect on the conductivity measurement. The supertonic transition was identified at temperature 235^{0c} to 270^{0c} of CDP/SDP/ZrO_2 composites under atmospheric pressure. Thermal stability of the solid acid composites such as the temperature of dehydration, melting, and decomposition was investigated under environments atmospheric humidification.

Keywords: Solid acid composite, conductivity, thermal analysis, caesium dihydrogen phosphate, fuel cell.

PVP varied BiOCl nano-crystals effective Photocatalytic Performance by Rhodamine B dye degradation under visible light

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Abstract

Now a days, Bismuth Oxyhalides (BiOX, X= Cl, Br & I) have materialize to an impressive aspirant for efficient photocatalytic deterioration of toxic pollutants and also for energy enhanced activity in numerous applications owing to its extremely crystalline constructions and an absolute electrical and optical properties. These nanomaterials can effectively degrade several types of organic, inorganic textile dyes and pharmaceutical effusions. However the various types of oxyhalides, Bismuth Oxychloride (BiOCl) perform layered tetragonal structure and p-type semiconducting nature and wide range of direct or indirect band gap values. In this work, the photocatalysts were synthesized by simple and facile hydrothermal method of bulk to nano materials, and the pure BiOCl materials faceted growth on the (00l) plane. Relevant molecular ratio used as the main precursors $\{Bi(NO_3)_3,5H_2O\}$ and HCl were applied to the hydrothermal condition in an oven for 3 hours at 160 ˚C with contained to addition of Polyvinylpyrrolidone (PVP) and citric acid as capping agents. The as-prepared simples were characterized by several techniques like as X-Ray diffraction (XRD), Field Emission Scanning Electron Microscopic (FESEM), UV-Vis spectroscopic and Raman analysis to approve proper evolution of the crystalline structures and phases, morphology, band gap and chemical bonds. The as-synthesized materials were exploiting for efficient deterioration of Rhodamine B dye under visible-light irradiations to inaugurate their usefulness for organic pollutant purification in aquatic medium.

Keywords: Bismuth Oxychloride, Polyvinylpyrrolidone, Photocatalysis, Rhodamine B, Visible light.

Performance of choline chloride based electrolytes in electrochemical double layer capacitors

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The need of renewable energy resources has emerged rapidly in previous decades due to increase in pollution and global warming by non-renewable resources of energy. However, energy storage devices can reduce these environmental hazards to great extent. The electrochemical double layer capacitor (EDLC) is one class of supercapacitor, which uses carbon electrode and stores energy with high power density. Different electrolyte materials including polymer electrolytes, aqueous electrolytes and lithium based electrolytes have been used in EDLC supercapacitors. In the present work, we have used activated carbon electrode and aqueous choline chloride (ChCl) electrolyte of different concentrations. We prepared 1 molar and 2 molar aqueous choline chloride electrolyte samples by simply weighing and dissolving choline chloride in water. The two supercapacitor cells were made using activated carbon electrode and two samples of electrolyte. The cyclic voltammetry, galvanic charge discharge and electrochemical impedance spectroscopy was recorded for these two supercapacitors. The specific capacitance for 1 molar ChCl based cell was found 408.5 mFg^{-1}@20mV/s and for 2 molar ChCl based cell was 520.8 mFg^{-1}@20mV/s using CV data. Choline chloride electrolyte also showed good electrochemical stability window of 0.8 V.

Keywords: Activated carbon, choline chloride, electrolytes, electrodes, EDLC capacitors.

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