International Conference
On
Energy Materials and Devices
(ICEMD-2022)
(January 11& 12, 2022)

Department of Physics (MMV)

Banaras Hindu University
Varanasi – 221005, India

Conference Website: https://icemd-2022.weebly.com

प्रो० विजय कुमार शुक्ल
कुलगुरू एवं
कार्यवाहक कुलपति
Prof. Vijay Kumar Shukla
Rector &
Officiating Vice-Chancellor

काशी हिन्दू विश्वविद्यालय
BANARAS HINDU UNIVERSITY

Telephone : 0542-2368938
Fax : 0542-2369100
Email : vc@bhu.ac.in
rector@bhu.ac.in
Website: www.bhu.ac.in

December 22, 2021

MESSAGE

I am happy to learn that Mahila Mahavidyalay, Banaras Hindu University is organizing an International Conference on “Energy Materials and Devices”.

The theme of the Conference is very relevant and I appreciate the organizers for selecting such a theme. I believe that this conference will be attended by experts from different branches of Physics and their lectures and deliberations on the topic will help in achieving fruitful scientific targets.

I extend my best wishes to the participants and wish the organizers all the best for grand success of the event.

(Vijay Kumar Shukla)

काशी हिन्दू विश्वविद्यालय
BANARAS HINDU UNIVERSITY

प्रो.अनिल कुमार त्रिपाठी, निदेशक, विज्ञान संस्थान
Prof. Anil Kumar Tripathi,
J C Bose National Fellow, FNA, FASc, FNASc, FNAAS
Professor, School of Biotechnology
Director, Institute of Science
Banaras Hindu University, Varanasi-221005

December 23, 2021

MESSAGE

I am happy to know that the Physics Section of Mahila Mahavidyalaya (MMV) is organizing an online "International Conference on Energy Materials and Devices". We all are aware that energy devices are the lifeline of our society as they are part of different electronic gadgets in daily life, health monitoring, and supporting systems. They also help in fighting atmospheric pollution by being an integral part of the electric vehicles, or exploring and realizing the optimal potential of renewable energy. I congratulate the organizing team to select such an important and relevant topic for the international conference.

It is the responsibility of the scientific community to come up with high-performing energy devices to meet the current demand. Such conferences bring the scientists of different expertise together resulting in well-targeted national/international collaborations. I convey my compliments and wish the conference and the organizing team a great success with fruitful outcomes.

(Anil K Tripathi)

Email:director.inst.science@gmail.com
tripathianil@rediffmail.com
Website: www.bhu.ac.in
Varanasi 221005, UP, India
T : 91-542-2369670
T : 91-8887161518

काशी हिन्दू विश्वविद्यालय
BANARAS HINDU UNIVERSITY
ESTABLISHED BY PARLIAMENT BY NOTIFICATION NO. 225 OF 1916

प्रो0 मधूलिका अग्रवाल
संकाय प्रमुख, विज्ञान संस्थान,
काशी हिन्दू विश्वविद्यालय
PROF. Madhoolika Agrawal
Dean, Faculty of Science, BHU

No. I.Sc./ Dean/ 2021-22/ Dated: December 20, 2021

MESSAGE

It is indeed a pleasure to learn that the Department of Physics, Mahila Maha Vidyalaya, BHU is organizing an online "International Conference on Energy Materials and Devices" during January 11 – 12, 2022. I am happy to note that an abstract is also being brought out to commemorate the occasion.

The focal theme of the ICEMD-2022; "Energy materials and devices" is very significant, considering the fact that energy devices are the life line of today's society. It is of paramount importance to develop new and cost effective materials and to understand the designing aspects. Such conferences will play an important role in achieving the new targets of energy demand of present society.

I am sure that the deliberations during the Panel Discussion with invited speakers from renowned international and national laboratories/ academic institution with the hope that the conference will initiate good collaborative works, and definitely would be prolific and the event would successfully achieve its goal. I wish the ICEMD-2022, a grand success, and best wishes for the entire endeavour.

MAgrawal

(Dr. Madhoolika Agrawal)
DEAN
Faculty of Science
Banaras Hindu University

Varanasi - 221005, UP, INDIA
Mob. : 8004930513
E : dean_sci@bhu.ac.in
W : www.bhu.ac.in

काशी हिन्दू विश्वविद्यालय
BANARAS HINDU UNIVERSITY
AN INSTITUTION OF NATIONAL IMPORTANCE ESTABLISHED BY AN ACT OF PARLIAMENT

महिला महाविद्यालय
MAHILA MAHAVIDYALAYA

डॉ० इनु मेहता
प्रोफेसर, अर्थशास्त्र विभाग
प्राचार्या

Dr. Inu Mehta
Professor of Economics
Principal

21.12.2021

Message

It is really a great pleasure for me that Department of Physics, Mahila Mahavidyalaya is organizing an online "International Conference on Energy Materials and devices" during 11-12 January, 2022. Due to Covid-19 pandemic the past two years have been really a tough time for human beings especially for academicians. Hence in order to maintain the pace of academic activities online Conference/Webinars are being organized throughout the world.

Energy devices are part and parcel of human life and fabrication of novel energy devices requires deep understanding regarding electrode materials, electrolyte materials and the techniques to fabricate the devices. I strongly believe that this conference will leave a special impact on our female students and motivate them to become true scientists. As the Principal of Mahila Mahavidyalaya, I appreciate the enthusiastic efforts of the entire organizing team and extend my best wishes for the successful completion of the conference.

Inu Mehta
Prof. Inu Mehta
Principal

BHU
capital of knowledge

Varanasi 221005, UP, INDIA
T : 91-542-2367927, 6701182
H : (542) 236766
E-mail Id: principalmmvbhu@gmail.com

काशी हिन्दू विश्वविद्यालय
BANARAS HINDU UNIVERSITY
AN INSTITUTION OF NATIONAL IMPORTANCE ESTABLISHED BY AN ACT OF PARLIAMENT

Dr. Neelam Srivastava, Professor of Physics
Convener ICEMD-2022
IQAC Coordinator-MMV
Professor-in-Charge Training and Placement cell (MMV)

From the Convener's Desk

In 1800, Volta introduced the concept of electric energy generation by keeping the paper/cotton cloth dipped in an electrolyte solution between piles of Copper and Zinc. Since then, energy devices have witnessed tremendous developments. They have become an inseparable part of our lives. Today, sustainable development in electronic technology demands an equivalent pace in the development of energy devices. The fast change in demand compels scientists to think of innovative methods and devise economical and environmentally admissible solutions to meet the demand.

The research in the field consists of various sub-fields and for a fruitful outcome, the fundamental understanding across all the domains is predominant, and collaborative research is essential. To this end, conferences provide a way to understand and discuss each other's research, leading to joint ventures. The platform it provides is crucial for furtherance in the research domain and the growth of researchers.

Innovations in the domain have continued to germinate in research labs situated across the globe. Although we faced time-zone restrictions while inviting the plenary/ invited speakers, we have tried to cover various backgrounds. The organizing committee is thankful to speakers who accepted our request even though it was odd hours for them. We hope that the new entrants in the field will be greatly benefitted by the conference, as it is designed to present the fundamentals of many important branches of energy devices on a single platform.

Considering the fact that, to accommodate good number of papers generally contributed papers don't get enough time to discuss their work, this conference has made special provision for contributed paper participants to make a separate 15 mins presentation for uploading it on the conference YouTube channel, besides their short presentation at conference. This not only ensures enough time to each of the participants to explain their work but also enables us to avoid parallel sessions. We are thankful to all the speakers and participants for their interest in ICEMD-2022.

Prof. Neelam Srivastava

BHU
capital of knowledge

Varanasi-221005, UP, India
T: 05426701066, M: +919415424782
W: http://srivastavaneelam.weebly.com
E: neelamsrivastava_bhu@yahoo.co.in, neel@bhu.ac.in

Conference Committee

Chief Patron

Vice-Chancellor, BHU

Patrons

Prof. Anil Kumar Tripathi

(Director, Institute of Science, BHU)

Prof. Madhoolika Agrawal

(Dean Faculty of Science, I. Sc., BHU)

Chairperson

Prof. Inu Mehta (Principal, MMV)

Conveners

Prof. Neelam Srivastava

Prof. Bhaskar Bhattacharya

Organizing Secretary

Dr. I. Panneer Muthuselvam

Treasurer

Dr. Manasi Ghosh

Advisory Committee

Prof Abdul K Arof, Malaysia
Prof. A.J. Pawlicka Maule, Brazil
Prof. Tan Winie
Prof. A. R. Kulkarni, IIT-B
Prof. D. Pandey, BHU
Prof. K. Shahi, IIT-K
Prof. R. K. Pandey, Amity Raipur
Prof. R. K. Sharma, IIT-Delhi
Prof. R. S. Tiwari, BHU
Prof. Rajiv Prakash, IIT-BHU
Prof. S.A. Hashmi, DU

Organizing committee

Prof. A. Dalvi, BITS-Pillani
Prof. A.K. Ghosh, BHU
Prof. Abhay Kumar Singh, BHU
Prof. Anchal Srivastava, BHU
Prof. Anji Reddy Polu, Hyderabad
Prof. Awalendra Kumar Thakur, IIT Patna
Prof. Diksha Katiyar, MMV-BHU
Prof. H. Mishra, MMV-BHU
Prof. Meenakshi Singh, MMV-BHU
Prof. Prabhakar Singh, IIT-BHU
Prof. Pramod Kumar Singh, Sharda, NCR Delhi
Prof. R.K. Singh, BHU
Prof. Shree Prakash Pandey, TMU, Moradabad
Prof. U. P. Singh, KIIT Bhuvneshwar
Dr. Acche Lal Saroj, BHU
Dr. Andrew Fanai, MMV-BHU
Dr. Manindra Kumar, DDU, Gorakhpur
Dr. Piyush Sonkar, MMV-BHU
Dr. Preetam Singh, IIT-BHU
Dr. Sailaja SahaSunkari, MMV-BHU
Dr. Swarnlata Singh, MMV-BHU

International Conference on Energy Materials and Devices
(ICEMD-2022)
(January 11& 12, 2022)

Technical Program

Day -1, 11th January 2022

9:15AM-10:35 AM
Inaugural Session

9:15 am: Digital floral tributes to our Visionary founder Bharat Ratna Mahamana Pt. Madan Mohan Malviya ji
9:20 am: BHU Kulgeet by MS. Poulomi Bhattacharya
9:30 am: Welcome Address by Chairperson (ICEMD-2022) and Principal (MMV) Prof. Inu Mehta
9:35 am: About the conference by Prof. Neelam Srivastava (Convener ICEMD-2022)
9:40 am: Address by Prof Madhoolika Agrawal, Special Guest and Dean (Faculty of Science)
9:45 am: Address by Prof. Anil Kumar Tripathi, Special Guest and Director (Institute of Science)
9:50 am: Inaugural Address by Chief Guest Dr. N Kalaiselvi, Director, CSIR-Central Electrochemical Research Institute (CSIR-CECRI), Karaikudi, India
10:20 am: Presidential remark by Prof V. K. Shukla (Rector and Vice-Chancellor Incharge)
10.30 am: Formal vote of thanks by Prof. Bhaskar Bhattacharya (Convener ICEMD-2022)

10:35 AM -11:20 AM
Keynote Talk

Sustainable Research approach for future Energy Storage devices
Dr. R. L. Sharma CEO-SPEL Technologies Pvt. Ltd. PUNE, India

Session-1
Chairperson-Prof. U. P. Singh

11:20 AM-11:55AM	Plenary	Dr. S Venkata Mohan, Senior Principal Scientist, IICT, Hyderabad	Microbial Electrochemical Systems with Multi-Facet Applications: Emerging Trends
11:55 AM-12:20 PM	I-2	Prof. Vellaichamy Ganesan, Department of Chemistry, Institute of Science, Banaras Hindu University, India	Highly Dispersed Metal Porphyrins/Phthalocyanines on Various Supports to Replace Pt-based Catalysts in Fuel Cells
12:20 PM-12:45 PM	I-10	Prof. Prabhakar Singh, Department of Physics, IIT (BHU) Varanasi, India	Bandgap Engineering and Its Applications

Session-2
Chairperson- Prof. Akhilesh Kumar Singh

12:50 PM-1:25 PM	Plenary	Dr. Venugopalan Srinivasan, Ex-Head, Battery Division, PSG, URSC, Bangalore	“Lithium Batteries: Present Scenario and Future Prospects”
1:25 PM-1:50 PM	I-3	Dr. A. Manuel Stephan, CSIR-Central Electrochemical Research Institute, India	Lithium-Sulfur Batteries: A Futuristic System

1:50 PM- 2:40 PM LUNCH

Session-3
Chairperson- Prof. Muhd Zu Azhan Yahya

2:40 PM-3:05 PM	I-1	Prof. S. A. Hashmi, University Of Delhi, India	Redox-Active Gel Polymer Electrolytes for High-Performance Carbon Supercapacitors
3:05 PM-3:30 PM	I-5	Prof. Vanchiappan Aravindan, Indian Institute of Science Education and Research (IISER), Tirupati, India	Research Progress on Li-Ion Capacitors

3:30 PM- 3:55 PM	I-6	Prof. Ravindra Kumar Gupta, King Saud University, Saudi Arabia	Cobalt-Based Solid Redox Mediators

Session-4

Chairperson-Prof. S. A. Hashmi

4:00 PM- 4:25 PM	I-7	Prof. Pramod Kumar Singh, Sharda University, India	Energy Devices Based on Waste Material Electrodes and Ionic Liquid Based Solid Electrolyte
4:25 PM- 4:50 PM	I-8	Prof. Muhd Zu Azhan Yahya, National Defence University of Malaysia	Effects Of Mo Substitution on Electrochemical Performance of Na3V2(PO4)3/C Cathode Composite For Sodium-Ion Batteries
4:50 PM- 5:25 PM	Plenary	Prof. Arumugam Manthiram, the University of Texas at Austin, USA	Sustainable Next-Generation Battery Technologies

Session-5

Expert Panel- Prof. M. V. Reddy, Prof. Prabhakar Singh, Prof. Yogesh Kumar, Prof Kamlesh Pandey, Prof. Sandeep Tomar, Prof. Ranveer Kumar

5:30 PM- 8:30 PM	Contributed Paper Oral Presentation Please See Annexure 1 of the Technical Session

International Conference on Energy Materials and Devices
(ICEMD-2022)

(January 11& 12, 2022)

Technical Program

Day -2, 12th January 2022

Session-6

Chairperson-Prof. Tan Winiie

9:30 AM- 9:55 AM	I-9	Prof. M.V. Reddy, Nouveau Monde Graphite (New Graphite World), Montréal, Québec, Canada	Recent Advances in Energy Storage Materials
9:55 AM- 10:30 AM	Plenary	Prof Xiulei "David" Ji, Oregon State University, USA	Ion Charge Carriers: Unlock the Potential of Storage Battery Chemistry
10:30 AM- 10:55 AM	I-4	Prof. Anshuman Dalvi, Birla Institute of Technology and Science Pilani, India	Solid Polymer Electrolytes Dispersed with NASICON Structured Nano-Crystallites for All-Solid-State Supercapacitor Applications

Session-7

Chairperson-Prof. Pramod Kumar Singh

11:00 AM- 11:25 AM	I-11	Prof. Tan Winie, Institute of Science, Universiti Teknologi MARA, Shah Alam Malaysia	Iron-Based Composite Electrode for Application in Supercapacitor
11:25 AM- 11:50 AM	I-18	Prof. Deepak Kumar, Faculty of Weapon Technology, Electronics and Mechanical Engineering School, Vadodara, India	Investigations On Glyme Based Na+ Conducting Polymer Gel Electrolytes for Electrochemical Applications
11:50 AM- 12:15 PM	I-13	Prof. Amit K. Chakraborty, National Institute of Technology Durgapur, India	Carbon Nanostructures for Electrochemical Supercapacitors
12:15 PM- 12:40 PM	I-14	Prof. Preetam Singh, IIT (BHU) Varanasi, India	Pseudocapacitive Metal-Carboxylate Electrodes for Hybrid Supercapacitors

12:40 PM- 1:30 PM LUNCH			
Session-8 **Chairperson-Prof. Anshuman Dalvi**			
1:30 PM- 1:55 PM	I-15	Prof. Udai Pratap Singh, School of Electronics Engineering, Campus-12, KIIT, Bhubaneswar-India	Advancement In Kesterite Based Thin-Film Solar Cells
1:55 PM- 2:20 PM	I-16	Prof. S. P. Pandey, Teerthanker Mahaveer University, Moradabad, U.P. (INDIA)	Solar Cell Technology: Optimization of Processing Parameters of Crystalline Si Solar Cells
2:20 PM- 2:45 PM	I-17	Prof. Kamlesh Pandey, University of Allahabad, India	Synthesis and Application of Polymer/Nanodiamond Composites
2:45 PM- 3:10 PM	I-12	Prof. Rajan Jose, Faculty of Industrial Sciences & Technology, Malaysia	Sustainable Materials & Processes for Electrochemical Capacitors
Session-9 **Chairperson- Prof. Amit K. Chakraborty**			
3:15 PM- 3:40 PM	I-19	Prof. Yogesh Kumar, ARSD College, University of Delhi, India	Advanced Electrode Materials for High-Performance Electrochemical Supercapacitors with Different Electrolytes
3:40 PM- 4:05 PM	I-20	Prof. Agnieszka Pawlicka, Universidade De São Paulo, Brazil	Eco-Friendly Polymer Electrolytes for Electrochromic Devices
4:05 PM- 4:30 PM	I-21	Prof. Diogo M.F. Santos, Instituto Superior Técnico, Universidade De Lisboa, Portugal	Towards Efficient Green H2 Production by Alkaline Water Electrolysis
4:30 PM- 4:55 PM	I-22	Prof. M. G. Buonomenna, Chemical Fundamentals of Technologies from the Italian Ministry for Instruction, University and Research (MIUR), Italy	Lithium-sulfur batteries: where are we now?
Session-10 **Expert Panel- Prof. Rajan Jose, Prof Preetam Singh, Prof. Mohan Lal Verma, Prof R. K. Gupta, Prof. S. P. Pandey, Dr. Piyush Kumar Sonkar**			
5:00 PM- 7:30 PM	Contributed Oral Paper Presentation Please See Annexure 2 Of the Technical Session		
7:30 PM	**Valedictory Function**		

Annexure 1: Oral Presentation Schedule of Contributed Papers

(All the oral presenters please remember that submitting a detailed video for Conference YouTube is must, only then your short (5min) presentation will be allowed here)

International Conference on Energy Materials and Devices **(ICEMD-2022)** (January 11& 12, 2022) Technical Program-Oral Presentation of Contributed papers **Day -1, 11th January 2022**					
Time Slot	Abstract Number	Your Name	Department	Institution	Title Of Abstract
5:30 PM	C1	Sanjit Kumar Rath	PG Dept. of Applied Physics and Ballistics	F M University, Balasore, India	Effective efficiency enhancement in Silicon Photovoltaics with alternative ARC and gettering
5:35 PM	C2	Shivaji Madhukar Sonawane	Physics	Bharatiya Jain Sanghatana’s Arts Science & Commerce College, Pune, India.	Characterization of ZnTe thin films prepared by cathodic electrodeposition as a back contact buffer layer to CdS/CdTe solar cells.
5:40 PM	C3	Dr. Harit Kumar Sharma	Physics	APS University Rewa, M.P.	Structural, optical and electrical properties of the ZnS and Zn1-xCdxS Nanoparticles for Solar Cell Application
5:45 PM	C4	Dr. A. L. Saroj	Physics	Science	Structural and ion transport study of CS-based Biopolymer electrolyte films
5:50:PM	C5	M.H. Priyad Arsini	PG Department of Applied Physics and Ballistics	Fakir Mohan University	Capacitance of ppy/rGo/Ni(OH)2 nanocomposite for supercapacitor applications
5:55 PM	C6	Ritu Singh	Chemistry	MMV, Banaras Hindu University, Varanasi-221005	Selective and sensitive determination of dual drugs on a molecularly imprinted polymer/ reduced graphene-modified electrode
6:00 PM	C7	Ankit Kargeti	Applied Sciences	BML Munjal University	Quantum chemical calculations on molecules with donor-π-acceptor structures for efficient Organic Field Effect Transistor
6:05 PM	C8	Jyoti Kumari	Physics	Banasthali Vidyapith	Investigation for Structural, Electronic and Optical characterization of lithium-based chalcopyrite semiconductors by using density functional theory

6:10 PM	C9	Vishal Rimal	Chemistry	Birla Institute of Technology, Mesra	Review on electrochemical kinetics of Carbon Dots
6:15 PM	C10	Dr. Meenal Gupta	Physics	Sharda University	Functional biochar derived from Desmostachya bipinnata for the application in energy storage/conversion devices
6:20PM	C11	Dr. Manmeet Kaur Bhuie	Applied Physics	Shri Shankaracharya Technical Campus, Bhilai	Heating effect, UV radiation and Trap depth parameters of rare earth doped Yttrium oxide for dosimetry applications
6:25 PM	C12	Bibek Kumar Sonu	Physics	Birla Institute Of Technology Mesra	Fast and stable electrolyte scandium co-doped barium cerate
6:30 PM	C13	Vishwa Pratap Singh	School of Material Science and Technology	Indian Institute of Technology(BHU) , Varanasi	Synthesis of H_2O_2 refluxed LaFeO3 loaded as filler in poly (vinylidene fluoride) for high energy density storage applications
6:35 PM	C14	Ms. Priyanka Lamba	Physics	Sharda University, Deshbandhu college (DU)	Simple and Rapid Ecofriendly Synthesis of NiO/RGO Nanocomposites using Guava Leaf Extract and their Physicochemical Characterization
6:40 PM	C15	Dr. B Keshav Rao	Applied Physics	Shri Shankaracharya Technical Campus	Structural, Electronic and Mechanical Properties of Hybrid h-BN/Graphene 2D layers: Density Functional Approach
6:45 PM	C16	Dhirendra Kumar	Chemistry	Shri Venkateshwara University	Synthesis And Characterization of Aryl Substituted 4 - Thiazolidino A,B – Unsaturated Ketones and Dimethyl amino Methylene Ketones And Their Biological Activity
6:50 PM	C17	Aparna Satish Ukarande	Department of Physics	Savitri bai PhulePune university	Impact of the bath temperature on CdTe thin films prepared by electrochemical technique
6:55 PM	C18	Dr Amit Saxena	Physics	Shri Vaishnav Vidyapeeth Vishwavidyalaya, Indore, India	Analytical Analysis of Concentration of Charge Carriers in Polymer Electrolytes Through Different Models
7:00 PM	C19	Pooja Rawat	Physics Department	Banaras Hindu University	AC conductivity and Ion dynamics behavior study of PVA based polymer electrolyte films
7:05 PM	C20	Prem Chandra Bharti	Physics	Indian Institute of Technology (BHU), Varanasi	Comparative study of Physical Properties of Cold-sintered CuPbBr3 and

					CuPbI3 Perovskite for Solar Cell Applications
7:10 PM	C21	Dr. SWETA SINGH	Physics	Mahatma Gandhi Central University	Synthesis, characterization, and energy storage application of carbon/graphene aerogel
7:15 PM	C22	Monika Vikal	Department of Environment Science	IGNOU, Delhi	Graphitic carbon nitride-based heterojunction nanocomposite for degradation of organic dyes
7:20 PM	C23	Subhrajit Konwar	Physics	Sharda University, India	Future Prospects of Biopolymer- Ionic Liquid Polymer Electrolyte
7:25 PM	C24	Swarnima Singh	Physics	Indian Institute of Technology (Banaras Hindu University) Varanasi	Structural and bandgap studies of Cs(Sn1/2Pb1/2)Br3
7:30PM	C25	Varsha Yadav	School of Applied sciences	Shri Venkateshwara University	Role of Natural Dye in Photovoltaic Performance of Dye Sensitized Solar Cell
7:35 PM	C26	Ashish Kumar Ranjan	Physics	IIT (BHU), Varanasi	Structural and Photo-conduction studies of NiO as a Hole Transport Material for Perovskite Solar Cells

Annexure 2: Oral Presentation Schedule of Contributed Papers

(All the oral presenters please remember that submitting a detailed video for Conference YouTube is must, only then your short (5min) presentation will be allowed here)

International Conference on Energy Materials and Devices
(ICEMD-2022)
(January 11& 12, 2022)
Technical Program-Oral Presentation of Contributed papers
Day -2, 12th January 2022

Time Slot	Abstract Number	Your Name	Department	Institution	Title of Abstract
5:00 PM	C27	Dr. Sujeet Kumar Chaurasia	Centre For Nanoscience and Technology	Veer Bahadur Singh Purvanchal University, Jaunpur	Impact of In-Situ Formed Silica Nanospheres on Physicochemical and Ionic Transport Properties Of PEO-Based Hybrid Electrolytes
5:05 PM	C28	Pawan Singh Dhapola	Chemistry	DSB Campus, Kumaun University, India	Development of porous carbon from Polyvinyl chloride (PVC) and its application in supercapacitor
5:10 PM	C29	Dr. Vijayeta Pal	School of Materials Science & Technology	Indian Institute Of Technology (Banaras Hindu University), Varanasi	Structural, Microstructure and Dielectric Properties of La2NiMnO6 Double Perovskites Ceramics
5:15 PM	C30	Manisha Chauhan	Physics	IIT (BHU), Varanasi	Influence Of Co-Doping on Structural, Morphological, And Electrical Properties Of Ruddlesden-Popper-Type Smsrnio4-δAs A Cathode Material For IT-SOFC
5:20 PM	C31	Raghubir Kumar Prajapati	Physics	Banaras Hindu University	To Study DC Conductivity And Dielectric Properties of Composition [PVA:CS:PEG]-Agno3 Based Biopolymer Electrolyte Films
5:25 PM	C32	Manisha Sharma	Physics	IIT BHU	Synthesis And Photoluminescence Studies of Lanthanide Doped Ca9Y(VO4)7 Polycrystalline Material
5:30 PM	C33	Uma Sharma	Physics	Indian Institute of Technology (BHU) Varanasi	Electrical Properties of Laxsr1-Xtio3-Δ As SOFC Electrode Material
5:35 PM	C34	Jyothy G Vijayan	Chemistry	M.S Ramaiah University of Applied Sciences	Synthesis and Characterization of Modified Moringa Olifera Seed Pod Nanocellulose Based Hydrophobic Polyurethane Xerogels

5:40 PM	C35	D. Lakshmi	Department of Physics	Bharathiar University	Backup Phase Assisted Mntio3 Electrodes for Supercapacitor Applications
5:45 PM	C36	Tabish Rasheed	Applied Science,	BML Munjal University	Design of Two Novel Dyes Having Maximum Absorption in Infrared Region: A DFT Investigation
5:50 PM	C37	Dona Susan Baji	Amrita Centre for Nano Sci. and Molecular Medicine	Amrita Vishwa Vidyapeetham, India	Rechargeable Alkali Metal Ion Batteries With Chemically Reduced Fe[Fe(CN)6] Cathode
5:55 PM	C38	SILPASRE E S J	Nano Energy Division	Amrita Center for Nanosciences and Molecular Medicine	Lithium-Rich Layered Cathode for Advanced Lithium-Ion Batteries – Particle Size and Operation Temperature Effects
6:00 PM	C39	Niti Agrawal	Physics	University of Delhi- Shyamlal College	Monthly Energy Yield Assessment of Solar Photovoltaic System Under Uniform Irradiance and Partial Shaded Conditions
6:10 PM	C40	Chandra Bhal Singh	School Of Materials Science and Technology	Indian Institute of Technology (B. H. U.), India	Band Gap Engineering of Batio3 Perovskite Oxide by Vanadium Doping and Observation of Photovoltaic Response
6:15 PM	C41	M Infanta Diana	Physics	Bharathiar University	Carbon Captivated Nasno2 Anode for Na-Ion Batteries
6:20 PM	C42	Ramesh A	Physics	Banaras Hindu University	Combustion Preparation of Reduced Graphene Oxide for Supercapacitor Application
6:25 PM	C43	Devesh Chandra Bharati	Department of Physics	Institute of Science, BHU, Varanasi	Effect of Ionic Liquid on Structural and Ion Transport Properties Of CS-PVA-NaI Based Biopolymer Electrolyte Films
6:30 PM	C44	Sachin Vijay Desarada	Department Of Physics	Savitribai Phule Pune University, Pune	Optimization of Mose2 Back Interface Layer for High Efficient CIGS Solar Cells: Numerical Analyses
6:35 PM	C45	Satyendra Kumar Satyarthi	Ceramic Engineering	Indian Institute of Technology (BHU)	Enhancement In the Dielectric Properties In Rare Earth Cerium Doped Linbo3 For High-Temperature Applications
6:40 PM	C46	Adlin Helen	Physics	Bharathiar University, India	Influence Of Filler Content on Magnesium Conducting Chitosan Biopolymer Electrolyte
6:45 PM	C47	Kamana Kumari Mishra	Physics	IIT (BHU), India	Catalytic Behaviour of Hydrothermal Processed NiO

6:50 PM	C48	T. Kiruthika	Department of Physics	Bharathiar University, India	One-Step Green Synthesis of Znfe2o4 Anodes for Li-Ion Batteries
6:55 PM	C49	Tejas Sharma	Department of Mechanical and Material Engineering	Universiti Tunku Abdul Rahman, Sungai Long Campus, Malaysia	Poly (methyl methacrylate) doped with ionic liquid for energy storage devices
7:00 PM	C50	Sushant Kumar	Physics	Sharda University, India	Preparation, characterization and application of low viscosity ionic liquid doped solid polymer electrolyte
7:05 PM	C51	Abhimanyu Singh	Physics	Gautam Buddha University	Electrical, Structural and Electrochemical performance of Polyethylene oxide doped with 1-ethy-3-methylimidazolium tricynomethanide ionic liquid
7:10 PM	C52	Dipti Yadav	Department of Physics (MMV)	Banaras Hindu University	Mg (ClO4)2 mixed crosslinked corn starch: A flexible and high conducting polymer-in-salt-electrolyte
7:15 PM	C53	Kalyan B. Chavan	Physics	Ahmednagar College	Structural and Optical Investigations on Direct current (DC) magnetron sputtered CZTS thin film
7:20 PM	C54	Diptarka Roy	Physics	Babasaheb Bhimrao Ambedkar University	Green synthesis of bismuth ferrite nanoparticle for PVA-PANI-BFO nanocomposite membrane to study the ionic conductivity with varying relative humidity

Ion Charge Carriers: Unlock the Potential of Storage Battery Chemistry

Xiulei "David" Ji

Oregon State University USA

Abstract

The design of storage batteries entails a holistic view. This talk will first summarize five considerations for the design of storage battery chemistries. Electrode materials and ion charge carriers are the reactants; electrolytes represent the reaction medium; battery operation fashions describe the reactors; the electrode-ion chemical bonding reflects the nature of the chemical reaction, which affects the thermodynamic and kinetic properties of batteries. The permutations of these five considerations result in ten unique approaches of studies. The chemical-reaction nature of batteries can be a vantage that unifies rather than compartmentalizes a new paradigm of storage battery research. I will cover four basic types of battery operation and summarize the evolution of battery chemistries with different cation and anion as charge carriers. I will illustrate the qualitative equations to estimate the operation potential of cation insertion or anion insertion in an electrode. Next, I will discuss the impacts of electrode-ion interactions on the kinetic properties of electrochemical reactions. Lastly, I will highlight the emerging types of concentrated electrolytes, particularly ZnCl2 molten hydrates, with respect to their ion speciation, water's O-H covalent bond, and implications.

Sustainable Next Generation Battery Technologies

Arumugam Manthiram

Walker Department of Mechanical Engineering
McKetta Department of Chemical Engineering
Materials Science and Engineering Program & Texas Materials Institute
The University of Texas at Austin

Abstract

Rapid increase in global energy use and growing environmental concerns have prompted the development of clean, sustainable, alternative energy technologies. Renewable energy sources like solar and wind are a promising solution, but battery technologies are critical to efficiently utilize electricity produced from them as well as for the electrification of transportation sector. Their widespread adoption, however, requires optimization of cost, cycle life, safety, energy density, power density, and environmental impact, all of which are directly linked to severe materials challenges. After providing an account of the current status, this presentation will focus on the development of advanced materials and new battery chemistries for near-term and long-term battery technologies. Specifically, the development of sustainable battery technologies, such cobalt-free lithium-ion batteries as well as sulfur-based lithium and sodium batteries that do not involve mining of transition metals, will be presented. An in-depth analysis of the degradation mechanisms with advanced characterization methodologies before and after extended cycling of the cells will be discussed.

Microbial Electrochemical Systems with Multi-facet Applications: Emerging Trends

Dr S. Venkata Mohan

Bioengineering and Environmental Sciences Lab, Department of Energy and Environmental Engineering, CSIR-Indian Institute of Chemical Technology (CSIR-IICT), Hyderabad- 500 007, India
E-mail: svmohan@iict.res.in; vmohan_s@yahoo.com

Abstract

Microbial electrochemical technology (MET) is emerging as a sustainable platform technology due to its inherent potential for diverse applications. Broadly, MET can be classified based on its applications viz. microbial fuel cell (MFC) for harnessing bioelectricity, bioelectrochemical treatment (BET) for waste remediation, bioelectrochemical systems (BES) or microbial electrosynthesis or electro-fermentation) for the synthesis of biobased products and microbial electrolysis cell (MEC) for H_2 production under applied potential. MFC primarily documented significant interest in the contemporary energy arena. BET with its good waste remediation capability is being pursued with great interest. Besides, BES which emphasizes on sequestering CO_2/waste for synthesizing value-added bioproducts is an emerging area of research. In this communication, an attempt will be made to present the progress made on MET research in our lab encompassing its application towards waste remediation and value-addition as focal objectives. Microbial catalyzed electrochemical reactions are the key which directly/indirectly are proportionally linked to electrometabolic activity of microorganisms towards final anticipated output. This communication is intends to document the current trends of MET towards multi-faced applications.

Lithium Batteries: Present Scenario and Future Prospects

Dr. S. Venugopalan

Ex-Head, Battery Division, PSG, URSC, Bangalore, India
Email: svenugopalan@pes.edu

Abstract

The role and development of advanced high energy and power density, long life, safer, cost-effective environmentally friendly lithium batteries is critical to the adoption of electric vehicles. Since its introduction and commercialization in 1991 by SONY Energetic many process innovation, material innovation, design modifications, optimization have taken place to simplify the process, minimize process time, material consumption, and improve process yield, performance, reliability, and reduce the cost of the cell. This has resulted in continuous improvement in the technology at a reduced cost. Threat to raw material availability, sustainability, and associated safety hazard aspects have influenced technological innovations. With rapidly expanding demand, batteries present a serious waste-management challenge in addition to safety hazards. The industry has addressed the growing need for better processes to manufacture and dispose of batteries as well as better ways to preserve virgin materials. This talk is intended to cover the current status of Lithium batteries, sustainability of the technology, medium, and long-term development directions will be illustrated with examples.

Redox-active Gel Polymer Electrolytes for High Performance Carbon Supercapacitors

S. A. Hashmi

Department of Physics and Astrophysics, University of Delhi, Delhi-110007, India
E-mail: sahashmi@physics.du.ac.in

Abstract

Supercapacitors, also referred to as electrochemical capacitors, store energy at the interfaces of electrolyte and solid phase electrodes (e.g. various forms of carbons) with high power density (5-10 kW kg-1) and long cycling life (105-106). Such devices are attractive as they are environment-friendly and cost-effective in the modern development, and perfect complementary technology to lithium-ion batteries for electrical vehicles (EVs) or hybrid electric vehicles (HEVs) [1].The electrical double layer capacitor (EDLC) is one type of supercapacitors, which employs porous carbon electrodes with large surface area and liquid or solid/polymer electrolytes. Carbons in different forms including graphene, CNTs, activated carbon, nano-fibres, etc. are used as capacitor electrodes due to their high surface area with controlled hierarchical porosity, etc.

The carbon supercapacitors or EDLCs show major limitation of specific energy (<10 Whkg-1). To enhance the specific energy of the devices, various approaches have been adopted, which include the use of suitable electrolytes, composite/hybrid electrodes and hybrid configuration.

Mostly liquid electrolytes are reported in the development of supercapacitors/EDLCs, which are plagued by limitations like leakage, corrosion, combustible reaction by-products and difficulty in proper handling. Recently, quasi-solid-state gel polymer electrolytes (GPEs) are being used on wider scale to circumvent such limitations. Recently, an important approach has been adopted to enhance energy density, in which small amount of redox additives (e.g. KI, NaI, hydroquinone HQ, etc.) are dispersed in liquid electrolytes or GPEs. The addition of redox-additive to the electrolytes leads to introduce additional pseudo-capacitance at the interfaces, responsible for capacitance, hence, energy enhancement.

This presentation would be devoted to fundamental aspects of supercapacitors, few approaches to enhance capacitance and hence, energy of devices along with few recent case studies carried out in our laboratory. The studies would be mainly dependent on electrochemical techniques including electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV) and charge-discharge tests. Few case studies would be presented on redox-active EDLCs based on activated carbon electrodes derived from biomasses and redox-active non-aqueous gel polymer electrolytes.

References:

[1] S.A. Hashmi, N. Yadav, M.K. Singh, in: Polymer Electrolytes: Characterization Techniques and Energy Applications, T. Winie, A.K. Arof, S. Thomas (Eds.), John Wiley & Sons, 2019, 231–297.

Highly Dispersed Metal Porphyrins/Phthalocyanines on Various Supports to Replace Pt-Based Catalysts in Fuel Cells

Vellaichamy Ganesan

Department of Chemistry, Institute of Science
Banaras Hindu University, Varanasi-221005, UP, India
E-mail: velganesh@yahoo.com and velgan@bhu.ac.in

Abstract

In electrocatalysis, the homogeneous distribution of catalysts plays a vital role in increasing the efficiency of the catalytic reaction. Carbon-based materials and ordered mesoporous silica are used as supports on which the catalyst can be dispersed uniformly. Metal porphyrins/phthalocyanines electro-catalyze several reactions including the oxygen reduction reaction. Four-electron reduction of oxygen which leads to the formation of H2O (or OH-) has high energy conversion efficiency and it is desired in fuel cells. Two-electron reduction of oxygen leads to the formation of H2O2 and has low energy conversion efficiency. Currently, in the fuel cells, Pt-based catalysts are used to realize the efficient four-electron reduction of oxygen. However, they are expensive and have stability issues. Developing a highly efficient and durable non-precious metal-based catalyst for the electrochemical reduction of oxygen can decrease the cost of fuel cells and ease the successful commercialization of devices based on fuel cells. Accordingly, the development of proficient inexpensive oxygen reduction catalysts is reported here. Metal porphyrins/phthalocyanines are incorporated into/onto various catalytic supports and the resulting materials are characterized by several techniques. Their catalytic efficiency is evaluated based on their oxygen reduction onset potentials. Ways to achieve the selective four-electron oxygen reduction are also discussed.

References:

[1] M. Pal and V. Ganesan, Langmuir, 2009, 25, 13264-13272.
[2] P. K. Sonkar, K. Prakash, M. Yadav, V. Ganesan, M. Sankar, R. Gupta, and D. K. Yadav, J. Mater Chem. A, 2017, 5, 6263-6276.
[3]. M. Yadav, P. K. Sonkar, K. Prakash, V. Ganesan, M. Sankar, D. K. Yadav, and R. Gupta, Int. J. Hydrog. Energy, 2020, 45, 9710-9722.
[4]. D. K. Singh, V. Ganesan, D. K. Yadav, and M. Yadav, Langmuir, 2020, 36, 12202-12212.
[5]. D. K. Singh, V. Ganesan, D. K. Yadav, M. Yadav, P. K. Sonkar, and R. Gupta, Catal. Sci. Tech., 2021, 11, 1014-1026.

Acknowledgments: IoE grant, BHU (scheme number: 6031).

Lithium Sulfur Batteries: A Futuristic System

A. Manuel Stephan

Electrochemical Power Sources Division
CSIR- Central Electrochemical Research Institute
Karaikudi 630 003, India
e-mail: amstephan@cecri.res.in or arulmanuel@gmail.com

Abstract

Although lithium -ion technology which employs layered $LiCoO2/LiFePO4$ cathode and carbonaceous anode separated by a porous polyolefin membrane soaked in a non-aqueous liquid electrolyte has found an inevitable niche in the consumer market toward powering portable electronic gadgets such as laptop computers, mobile phones, the limited topotactic chemistry impedes enhancement of energy and power density. Besides its high cost and poor safety issues have been a driving force for researchers to explore beyond the current state-of-the-art lithium-ion-battery technology for large-scale applications such as electric-mobility and stationary power storage devices. The unique properties such as high abundance of sulfur, relatively low mass, and high theoretical capacity of 1672 mAh g−1makes lithium−sulfur (Li−S) batteries a promising successor to meet out the aforementioned energy demands. It is also worth mentioning that the Gibbs energy of the Li−S reaction is about 2600 Wh kg−1, which is almost five times higher than the theoretical energy density of a Li-ion system.

Despite these advantages, the efficient utilization of Li–S batteries is yet to be realized due to several challenges including the poor electronic conductivity of sulfur (5 x 10-27 S cm_1 at 30 °C) and rapid deterioration of the lithium anode surface due to repeated deposition and stripping, as well as the formation and subsequent shuttling of polysulfides between electrodes.

One very promising method of overcoming this shortcoming is by employing a sulfur cathode with high sulfur loading in conjugation with interlayers or modified separators which would prevent polysulfide shuttle. The permselective separator is a modified separator made by coating the conventional separator with a permselective material which is capable of mitigating polysulfide shuttle. In the present work, permselective membranes have been prepared by coating various oxide/metal organic frameworks/ porous organic frameworks on the conventional porous polypropylene separators and introduced between the electrodes for lithium sulfur cells. The introduction of permselective membranes has successfully prevented the self-discharge of lithium sulfur batteries and improved their performances significantly.

References:

1. S. Shruti, A. Manuel Stephan, ACS Applied Energy Materials. 2020, 3, 8095−8129
2. S. Shruti, N. Angulakhsmi, H. Alkordi, A. Manuel Stephan, J. Mater. Chem A.,6 (2018) 14623-14632

Solid Polymer Electrolytes Dispersed with NASICON Structured Nano-Crystallites for All-Solid State Supercapacitor Applications

Anshuman Dalvi

Department of Physics
BITS Pilani India-333031
Email: adalvi@pilani.bits-pilani.ac.in

Abstract

After a significant work on liquids, gels as electrolytes, there has been a considerable attention towards supercapacitors with a ‘solid state electrolyte’. This is because, use of liquids/gels limits mechanical/thermal stability. To realize a liquid free all-solid-state supercapacitors (ASSCs) this work has been planned. Using NASICON structured Li+ ion conductor LATP composite solid electrolytes with high ionic conductivity were developed by a milling assisted synthesis route. LATP reinforced PEO- LiX (X = ClO^{4-}, $TFSI^{-}$, $CF_3SO_3^{-}$) composite solid polymer electrolyte (CSPE) membranes were prepared by milling assisted route, and directly used for ASSCs. A hot-roll lamination technique was used for the electric double-layer capacitor (EDLC) cells fabrication in which high surface area activate carbon (~ 800-1000 m2g-1) was used as electrodes. The EDLCs display appreciable specific capacitance of ≥100F/g at 40°C ~1Ag-1 and 2V. The content of conductive fillers is seen to play an important role in the performance. Some of these solid-state EDLCs at 40°C exhibit stability up to ~16000 cycles with appreciable coulombic efficiency and capacity retention. Interestingly, the electrode-electrolyte (solid-solid) interface remains quite stable after the charge-discharge cycling. Present investigation suggest that with an ionic conductivity of ~ 10^{-4}□-1cm^{-1} in the solid state, it is possible to form electric double layer capacitors suitable for low power applications. However, enormous efforts are required to enhance the performance parameters, which are currently limited due to interfacial issues.

Research Progress on Li-ion Capacitors

Vanchiappan Aravindan*

Department of Chemistry, Indian Institute of Science Education and Research (IISER), Tirupati-517507
*Email: aravindan@iisertirupati.ac.in

Abstract

Hybrid electrochemical capacitors or Li-ion capacitors (LIC) is a hybridization of Li-ion battery (LIB) and electric double-layer capacitors. As a result, the new configuration is anticipated to deliver high energy like LIB and high power like supercapacitors. Similar to LIB systems, the carbonaceous negative electrodes are used in the pre-lithiated form, whereas activated carbon (AC) remains a popular candidate for the counter side. However, in reality, the LIC assembly failed to translate desired energy and power densities. The modification of the AC electrode does not fulfill our requirements, which provides only the marginal improvement. Therefore, the only way to increase the charge-storage capability is the modification in the battery type component. Generally, the battery type component will be classified into three categories, viz. insertion, alloying, and conversion. In my talk, I will talk briefly about how the different mechanisms are employed in the LIC assembly with suitable examples. Also, highlight the possibility of utilizing two mechanisms together for the betterment of the system.

Keywords: Battery; supercapacitor; energy; power; intercalation.

Cobalt-Based Solid Redox Mediators

Ravindra Kumar Gupta

King Abdullah Institute for Nanotechnology, King Saud University, Riyadh 11451, Saudi Arabia
Email: rgupta@ksu.edu.sa Contact Number: +966-597546514

Abstract

The regions lying near to and between the Tropics of Capricorn and Cancer possess high sunlight irradiance from 1.6 to 2.5 MWhm-2. Dye-sensitized solar cell (DSSC)is being considered one of the highly attractive and fascinating renewable energy sources for electricity generation. A DSSC utilizes, in general, a highly conducting I─/I_3^- redox mediator, which inhibits back electron transfer reactions, regenerates dyes via the oxidation of I─ into I_3^- at the working electrode, and reduces I_3^- into I─ at the counter electrode. In the presentation, we will discuss cobalt-based solid redox mediators. The Co2+/Co3+ redox couple-based electrolytes offer several advantageous properties over the I─/I_3^--based electrolytes. The solid nature of the redox mediator makes the device economical, easy in processing and manufacture, and sustainable in harsh environmental conditions. We have synthesized new solid electrolytes using a lithium salt, LiX (X = TFSI or Tf); cobalt salts, Co(bpy)3(TFSI)2 and Co(bpy)3(TFSI)3; and a solid matrix, succinonitrile, poly(ethylene oxide), or succinonitrile-poly(ethylene oxide) blend. Succinonitrile is a nonionic and low-molecular-weight plastic crystal with a low melting temperature, high dielectric constant, and waxy nature, which make this a solid plasticizer. Its nitrile group offers transport of a cation. Poly(ethylene oxide) is a natural choice as a matrix because of its self-standing film formation property, thermal stability up to 200^0C, ecological, biodegradable, economical, dielectric constant between 4 and 8 for ionic salt dissociation, the segmental motion of polymer chains, ion transport through ethereal oxygen, and just the right spacing between coordinating ethereal oxygens for maximum solvation of the cations by the (□CH2□CH2□O□) mer. The blend combines the beneficial properties of both succinonitrile and poly(ethylene oxide). We have discussed the electrical transport, structural, optical, and thermal properties of solid electrolytes and compared them with those of liquid electrolytes prepared identically using acetonitrile.

Keyword: Dye-sensitized solar cell, PEO, Succinonitrile, Electrical Conductivity, FT-IR

Energy Devices Based on Waste Material Electrodes and Ionic Liquid Based Solid Electrolyte

Pramod K. Singh

Head, Center of Excellence on Solar Cells & Renewable Energy, Department of Physics, School of Basic Sciences & Research, Sharda University, Greater Noida 201310, India
E-mail: pramodkumar.singh@sharda.ac.in,
OrcidID:http://orcid.org/0000-0002-3155-6621?lang=en#sthash.VyzdlgSV.dpuf,
Contact No.: +91-9971729840

Abstract

During Covid pandemic situation world has moved to develop environmentally safe materials also known as green materials. Moving ahead, we have tried to develop plastic waste-based Carbon as electrodes and safe ionic liquid (IL) doped polymer electrolyte. Porous Carbon materials has been developed using plastic bottle throne within campus of Sharda University while variety of low viscosity ionic liquids and Polyethers have tested. These polymer electrolytes are characterized by impedance spectroscopy, optical microscopy (OM), differential scanning calorimetry, x-ray diffraction (XRD), and fourier transform infrared spectroscopy (FTIR). Finally, we have tested these Carbon-based electrodes and IL doped high conducting solid polymer electrolyte films in energy devices namely supercapacitors and dye sensitized solar cell.

Keywords: İonıc Liquid, Polymer electrolyte, Supercapacitor, Dye sensitized solar cell

Effects of Mo Substitution on Electrochemical Performance of Na3V2(PO4)3/C Cathode Composite for Sodium-Ion Batteries

M.F. Rosle[a,c], F.W. Badrudin[b], S.M. Hasanaly[a,c], S.A.M. Noor[b], A.H. Hashim[c], M.Z.A. Yahya[a*]

[a]Faculty of Defence Science and Technology, National Defence University of Malaysia,
57000 Kuala Lumpur, Malaysia
[b]Centre for Defence Foundation Studies, National Defence University of Malaysia,
57000 Kuala Lumpur, Malaysia
[c]Industrial Center of Innovation in Energy Management, SIRIM Industrial Research, Kulim Hi-Tech Park, 09000
Kulim Kedah, Malaysia

Abstract

NASICON-structure of Na3V2(PO4)3/C (NVP/C) exhibits excellent Na+ insertion-extraction capability, however suffered from volume change and low electronic conductivity. Series of Na3V2-xMox(PO4)3/C ($0\leq x \leq 1$) synthesized by the self-catalyzed sol-gel route has been investigated to suppress these issues. Both experimental and DFT results confirm the Mo6+ substitution via partial replacement of the V3+site resulting in significant electrochemical effects. The shift of X-ray-diffraction patterns is observed as the substitution amount exceeds the solid solubility limit leads to the alteration of the rhombohedral NVP/C structure. The optimized Na3V2-xMox(PO4)3/C exhibits high discharge capacity with a small variation of lattice parameters and volume changes upon extraction of two Na+ per formula unit. Among those series, Na3V1.7Mo0.3(PO4)3/C demonstrates the highest specific capacity of 122 mAh g-1at 0.2C correlates to the optimum kinetic response. Two potential discharged plateaus are observed at 3.4V and 1.6V (vs. Na+/Na), corresponding to the V3+/V4+ and V2+/V3+ redox couples activities respectively. Interestingly, Na3V1Mo1(PO4)3/C corresponds to the highest Mo6+ concentration exhibits an extended voltage plateau in the low voltage region at 1.6 V which promising as an anodic electrode for Na-ion batteries.

Keywords: Sodium-ion batteries; Na3V2-xMox(PO4)3/C; Mo-substitution; Rhombohedral NASICON

Recent Advances in Energy Storage Materials

M.V. Reddy

Noveau Monde Graphite, Montreal, Quebec, Canada
E-mail: reddymvvr@gmail.com

Abstract

Lithium-ion batteries (LIBs) are used in present-day portable electronic devices, electric/hybrid electric vehicles and back-up power supplies. Further, LIBs need to satisfy several criteria, namely, cost-reduction, improvement in energy density, safety-in-operation at high current rates, and improvement in the low-temperature operation. To satisfy the above criteria, research is being carried out worldwide to find alternative novel electrode materials for batteries, improved the performance by various materials synthesis process, surface modification, and fabrication technology.

In my talk, I will discuss our studies on novel metal oxides, nitrides, fluorides and graphene/metal oxide composite electrode materials related to energy storage. Specifically, I will focus on materials, such as LiMPO4F (M= V, Fe),novel V-based metal-organic framework materials oxalato Phosphate, Phosphite cathodes, Mo-metal clusters, and Sn-based hollandties and Sn-Pyrochlore type structure, metal fluorides and oxyfluorides, Nano- M N, O (M=Co,Ni, Cu, Mn) and, materials processing, characterization techniques, fundamentals, interface studies and applications related to energy storage. Various preparation methods (Molten salt, Graphenothermal/carbothermal, coprecipitation, Hydrothermal, Combustion, Ball-milling, solgel and Nitridation, fluorination), Solid electrolytes sintering techniques by powder metallurgy techniques, and thin films fabrication and surface coating techniques. Prepared materials were characterized by Rietveld refinement X-ray diffraction, Neutron diffraction, Rutherford backscattering spectrometry (RBS), Nuclear reaction (NRA), AES, X-ray absorption/photoelectron spectroscopy (XAS/XPS), SEM, TEM, Raman/IR, density and BET surface area methods. Electrode fabrication and various electroanalytical studies like cyclic voltammetry, galvanostatic cycling, and electrochemical impedance spectroscopy, GITT, PITT techniques for Li, Na, K-ion batteries, and in situ and ex-situ studies, reaction mechanisms, and voltage hysteresis and present challenges will be discussed.

Keywords: Materials Synthesis; Energy storage; cathode; anodes; characterization; Electrochemical Properties

References:

1. M.V. Reddy, C.M. Julien, A. Mauger, K. Zaghib, Sulfide and oxide inorganic solid electrolytes for all-solid-state Li batteries: A review, Nanomaterials, 10 (2020) 1606.
2. M.V. Reddy, M. V.; G.V. Subba Rao, B.V.R. Chowdari, "Metal oxides and oxysalts as anode materials for lithium-ion batteries" Chem. Rev. 113 (2013) 5364. (2640 citations)
3.More details of publications are listed inhttp://scholar.google.com.sg/citations?user=pWKr2M0AAAAJ&hl=en ;Orcid ID: 0000-0002-6979-5345

Band Gap Engineering and its Applications

Prabhakar Singh*

Department of Physics, Indian Institute of Technology(Banaras Hindu Universities) Varanasi, Varanasi (U.P)
*Email: psingh.app@iitbhu.ac.in

Abstract

Band gap engineering is controlled manipulation of band gap of the materials/meta-materials to get desired properties. The electrical and optical properties of materials are significantly affected by band gap tuning; therefore, band gap engineering is a powerful technique for designing the electronics and optoelectronic devices. With progress in science, the band gap engineering is not limited to electronic devices only; rather it has been extended to photonic and phononic devices. Along with meta-materials, novel synthesis techniques provide novel band structured devices. In this presentation, along with the general descriptions of band gap engineering and its applications, a few works from my laboratory will also be briefed. My research group actively works on materials Physics for energy applications. Our research interest is materials for fuel cell, photovoltaic cell, and Hydrogen/Oxygen generation. I will discuss band gap alteration behaviour for some of transition metal oxide, Perovskite oxides and halides with its implications on optoelectronic as well as interdisciplinary electrochemical properties. The orientation and thickness alteration of ZnO thin films altered the band gap to solar blind region as confirmed through both the experimental and theoretical results. Further, we designed the 1D photonic meta-surfaces of TiO2 with reduced graphene oxide with an attempt to obtain broader absorption bandwidth in NIR. The experimental and numerical simulation results suggest phonon scattering dominated free carrier absorption in NIR. Our studies implicate that band gap engineering along with doping strategies play a crucial role for materials physics.

Iron-Based Composite Electrode for Application in Supercapacitor

Akmal Arsyad[a], FarishIrfalSaaid[a], M. Rusop[a], Amit Kumar[b], Tseung-Yuen Tseng[b], Tan Winie[a,c*]

[a]Center for Functional Materials and Nanotechnology, Institute of Science, Universiti Teknologi MARA, 40450
Shah Alam, Selangor, Malaysia
[b]Institute of Electronics, National Chiao-Tung University, 1001 Ta Hsueh Rd, Hsinchu 300, Taiwan
[c]Faculty of Applied Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia
*Corresponding Author: tanwinie@uitm.edu.my

Abstract

Different morphologies and sizes of iron cobaltite have been prepared by a simple hydrothermal route. The dependence of electrochemical properties on the morphology and size of iron cobaltite has been investigated. The optimized structure of iron cobaltite was then added with different amounts of multi-walled carbon nanotubes (MWCNTs). The effect of MWCNTs was investigated using X-ray diffractometer (XRD), nitrogen absorption/desorption, field-emission scanning electron microscope (FESEM) and high-resolution transmission electron microscopy (HRTEM). The electrochemical properties of iron cobaltite/MWCNTs were examined by cyclic voltammetry (CV), galvanostatic charge/discharge (GCD) and electrochemical impedance spectroscopy (EIS) in an aqueous 6 M KOH. An asymmetric supercapacitor was fabricated with iron cobaltite/MWCNTs as the cathode and activated carbon as the anode. The supercapacitor exhibited maximum power density of ~3100 W kg-1 and maximum energy density of ~38 Wh kg-1. It demonstrated 80 % capacitance retention after 2000 cycles.

Keywords: Iron cobaltite, Composite, Electrode, Hydrothermal, Supercapacitor

Sustainable Materials & Processes for Electrochemical Capacitors

Rajan Jose

Nanostructured Renewable Energy Materials Laboratory, Faculty of Industrial Sciences & Technology, Universiti Malaysia Pahang, 26300 Kuantan, Malaysia; rjose@ump.edu.my

Abstract

Emergence of sustainability as the new normal and consequent concerns over material sustainability for various industrial sectors accelerated materials discovery process from renewable sources [1,2]. Energy storage become one of the dominant industries currently and most of the high performing energy storage devices such as lithium ion batteries use expensive mined materials as electrodes with enormous processing and value addition. Biomass derived carbon has been suggested as a possible material for energy storage, however, they mainly suffer from lower performance indicators [3-4]. We have explored augmenting properties of biomass carbon with small amounts (~5 – 10 wt.%) of metals or metal oxides to enhance the charge storage parameters in lithium-ion capacitors, battery–supercapacitor hybrids, and electrochemical capacitor storage modes besides developing eco-friendly and green routes for their processing using physical means than chemical methods. Four strategies were adopted: (i) enhancing the charge storage sites by filling large voids in porous carbon by hierarchical 3D nanoflowers or composite nanostructures [5-7], (ii) developing a thin metal oxide film over porous carbon surface through a simultaneous activation and coating process [8], (iii) developing a thin metal film over porous carbon [9], and (iv) green reduction of graphene oxide to reduced graphene oxide by means of physical methods than chemical ways [10,11]. Several advanced carbon structures are thereby synthesized; in supercapacitive charge storage mode they gave charge storability of ~60% of lithium battery and ~10 times more power capability than lithium battery. Only 10% metal compositions could boost up the energy storage capabilities dramatically. Promising green processing routes are also developed which avoid large scale toxic chemicals for developing advanced materials.

References:

1. R. Jose and S. Ramakrishna, Materials Circular Economy, (2021), 3, Art. No. 1.
2. S. Ramakrishna and R. Jose, Sci. Total Environment 806 (2022), 151208.
3. I. I. Misnon, NKZ Zain, R. A. Aziz, B. Vidyadharan, R. Jose Electrochimica Acta, 174, (2015)78
4. I.I. Misnon, NKM Zain, R Jose, Waste and Biomass Valorization, (2019)10, 1731-1740
5. B. Pal, S.G Krishnan, B. L. Vijayan, M. Harilal, C.C. Yang, F. I. Ezema, M. M. Yusoff, R. Jose, J Electroanal. Chem. (2018) 817, 217-225
6. B.L. Vijayan, N.K. Mohd Zain, I.I. Misnon, M.V. Reddy, S. Adams, C.C. Yang, G.M. Anilkumar and R. Jose, Energy & Fuels, (2020) 34, 5072-5083.
7. BL Vijayan, II Misnon, GM Anilkumar, CC Yang, R Jose, J. Alloys Compd. (2021) 858, 157649
8. B. L. Vijayan, I. I. Misnon, G. M. A. Kumar, K. Miyajima, M. V. Reddy, K. Zaghib, C. Karuppiah, C.C. Yang, R. Jose, J. Colloid and Interface Sci. (2020), 562, 567-577
9. BL Vijayan, II Misnon, C Karuppaiah, GMA Kumar, S Yang, CC Yang, R. Jose, J. Power Sources (2021) 489, 229522
10. A Yar, JO Dennis, MSM Saheed, NM Mohamed, M I Irshad, A. Mumtaz, R. Jose, J. Alloys Compd. (2020) 822, 153636
11. A Yar, JO Dennis, A Yasin, FU Din, M Irfan, MS Khan, CC Yang, R Jose, Sustainable Energy & Fuels 5, (2021)2724-2733

Carbon Nanostructures for Electrochemical Supercapacitors

Amit K. Chakraborty[a,b]

a-Carbon Nanotech. Lab, Department of Physics, NIT Durgapur, Durgapur-713209, India
b-Centre of Excellence in Advanced Materials, NIT Durgapur, Durgapur - 713209, India.
*E-mail: amit.chakraborty@phy.nitdgp.ac.in

Abstract

Technologies for storage of electrochemical energy has received enormous research attention in recent years due to rapid industrialization and increasing energy consumption across the globe. Transition metal compounds (TMC) such as their hydroxide, oxides, sulfide are well known pseudo-capacitive materials used for electro-chemical capacitors. However, absence of redox active groups and poor electrical conductivity often limits their performance which can be improved by combining them with different carbon nanostructures (CNS) such as carbon nanotube (CNT), graphene, reduced graphene oxide (RGO), etc. due to their excellent electronic property as well as mechanical and chemical stability.

In this paper, I shall present our approaches of combining metal hydroxides/oxides with various CNS and demonstrate how they improve the electrochemical energy storage properties. In addition, I shall also show that doping with cations is another way by which the electrochemical properties of the electrode materials to be used for supercapacitor can be improved. Some of the electrodes developed by us showed specific capacitance values in excess of 2000 F/g along with more than 80% charge retention upon 10000 cycles which are comparable or better than contemporary literature.

Reference:

[1] N Chakrabarty, AK Chakraborty, H Kumar, The Journal of Physical Chemistry C 123 (48), 29104-29115, 2019
[2] N Chakrabarty, A Dey, S Krishnamurthy, AK Chakraborty, Applied Surface Science 536, 147960, 2020
[3] N Chakrabarty, M Char, S Krishnamurthy, AK Chakraborty, Materials Advances 2 (1), 366-375, 2021
[4] N. Chakrabarty, A.K .Chakraborty, Electrochim. Acta, vol. 297, pp 173-187, 2019

Pseudocapacitive Metal-carboxylate Electrodes for Hybrid Supercapacitors

Dr. Preetam Singh

Assistant Professor
Dept. of Ceramic Engineering
IIT (BHU) Varanasi

Abstract

To overcome the environmental challenges caused by utilization of fossil fuel based energy technologies, coupling of renewable sources such as sources such as solar, wind and tidal with high power and high energy density containing large scale electrochemical energy storage devices are important to harness the electricity at fix current and voltage; a key requirement of electrical appliance and electronics. Energy storage process at electrode surface occurs differently depending on the interaction occurring at electrode surface between electrode and electrolyte such as EDLC, surface redox and intercalation of ions. EDLCs (Electric Double Layer Capacitors), also known as supercapacitors or ultracapacitors, offer another solution to ensure quality and short-term reliability in power systems. Like a conventional capacitor, electricity in an EDLC is stored in the electrical field between separated plates; the capacitance is a function of the plates' area, the distance between them, and the dielectric constant of the separating medium.

The Faradaic charge transfer due to very fast sequence of reversible redox, electro-sorption or intercalation processes on the surface of suitable electrodes called pseudo-capacitance that results high degree of electrochemical charge storage than EDLC. In simple term pseudo-capacitor can be understand as battery type capacitors. Pseudocapacitive electrode in the form of asymmetric supercapacitors can provide simultaneous solution for high power delivery as well as superior energy storage. Metal-organic frameworks (MOFs) are open framework structures where materials are constructed by joining metal-containing units with organic linkers creating permanent porosity. We have also focused our research in development of high power high energy density batteries; in turn, we have extended our studies on aqueous electrolyte based pseudo-capacitor electrodes. We have envisaged metal oxalates as potent pseudo-capacitor electrodes due to its open pore framework structure with superior structural stability and accessibility of $M^{2+/3+/4}$ redox energies. Recently, we have developed anhydrous CoC_2O_4 nanorod as potential energy storage electrode that showed superior specific capacitance equivalent to 2116 F/g at 1A/g in the potential window of 0.3V was observed for anhydrous CoC_2O_4 nanorods in aqueous 2M KOH electrolyte. In full cell asymmetric supercapacitors (ASCs) mode in which anhydrous CoC_2O_4 nanorod was made as positive electrode and Activated Carbon (AC) utilized as negative electrode within an operating potential window of 1.3V, highest specific energy of 129Wh/kg and specific power of ~647W/kg at 0.5A/g current density was obtained with superior cyclic stability. The energy and power values reported here are few times higher than those of lead-acid batteries banned in western world (Europe and America) due to high toxicity of lead (Pb).

Advancement in Kesterite Based Thin-Film Solar Cells

Udai P. Singh

Thin Film Photovoltaic Lab, School of Electronics Engineering,
Kalinga Institute of Industrial Technology (Deemed to be University)
Bhubaneswar-751024 (India)
*Email: singhup@kiit.ac.in

Abstract

In thin film solar technology, Kesterite (Cu_2ZnSnS_4) based absorber layer is one of the most attractive technology due to low toxicity and large availability of its constituent elements. It is a P-type direct band gap material with high absorption coefficient (>104 cm^{-1}). The band gap of Kesterite material varies between 1 to 1.5 eV with the variation in Se and S in the composition of CZTSSe. The maximum power conversion efficiency obtained at lab scale is 12.6% reported in 2014 using Hydrazine-Based solution technique. It has to go long way to compete with the well-established CIGS and CdTe based thin film solar cells.

Several studies have happened to increase the efficiency beyond 12.6%. But the challenging task is to control the growth and defect formation during formation of the films. Variations in the composition lead to the formation of intrinsic point defects (anti-sites, vacancies and interstitials) and deep level defects in the Kesterite material resulting in degradation in the Voc and carrier lifetime.

To increases, the efficiency of the CZTS/Se based solar cell, many researchers started doping and alloying with different element to improve its electrical, electronic, interface and charge transport properties. Doping with alkali metal increases the grain size and in turn improves the optoelectronics properties of CZTS/Se. Among all the alkali metal doping with Li shows better efficiency of 11.1%. One of the most studied methods is partial replacement of Cu by Ag. In CZTSSe alloying with Ag reduce the CuZ nantisite defects, increase the distance between conduction band and Fermi level and the mobility. The maximum efficiency of ACZTSSe reported is 11.83%. Ge is one of the most suitable and favorable elements in doping and alloying with Kesterite material. Ge substitution in CZTSSe partially and dully replace the Sn. Doping with Ge improve the grain size, surface morphology and reduce the Sn related deep defects and Voc deficit. The maximum efficiency of Ge alloyed CZTSSe based solar cell reported is 12.3%. There are many other elements used for doping and alloying viz Si, Mg, Sb, Mn etc. to improve the efficiency of CZTSSe based devices.

In the present presentation, we will discuss the advancement and limitation of Kesterite based thin film solar cells and its future prospects.

Keywords: Kesterite based solar cells, Thin-film, Efficiency, Defects, doping

Solar Cell Technology: Optimization of Processing Parameters of Crystalline Si Solar Cells

S.P. Pandey

Department of Physics, Teerthanker Mahaveer University, Moradabad
Corresponding Author: pandeysp72@gmail.com

Abstract

The demand for energy is increasing steadily and rapidly worldwide. However, the conventional sources of energy such as fossil and nuclear fuels are limited. Moreover, the associated negative effects on the environment such as the greenhouse effect, the hole in the ozone layer, acid rain and smog can no longer be neglected. Therefore, the conversion of sunlight into electricity using photovoltaics (PV) is a very attractive way to produce renewable energy. Silicon solar cells are still in demand for the researchers to use as a photovoltaic system. PV competes with the conventional energy since the production cost of electricity from it is still higher compared to the traditional methods. Therefore, the aim of most of the research is to increase the competitiveness of photovoltaics. The cost of solar cell can be reduced either by reducing materials and their processing cost or by increasing the efficiency of it.

In the present work an effort has been devoted to optimize the process involved to develop the high efficiency silicon solar cells. A comparative study has been taken for the silicon solar cell of boron and Al BSF layer in terms of cell parameters. Boron is the attractive candidate for a BSF layer because of many advantages over Al BSF layer in a silicon solar cell.

Keywords: Doping, Back surface field, Rapid Thermal Process, Texturing, Sputtering,

Synthesis and Application of Polymer/Nanodiamond Composites

Kamlesh Pandey and Mrigank Mauli Dwivedi

National Center of Experimental Mineralogy and Petrology,
University of Allahabad Allahabad-211002,U.P., India
Email: kamleshpandey@allduniv.ac.in

Abstract:

Nanodiamond (ND), an allotrope of carbon nanomaterials which offers diamond properties in nanometer scale, was first discovered in the 1960s. Nanodiamond (ND) possess unique spherical shape containing diamond-like structure at the core with graphitic carbon outer shell which intuitively contains many oxygen-containing functional groups at the outer surface. The solution mixing technique has been widely used to prepare uniform dispersion of ND in various polymers such as poly vinyl alcohol (PVA), chitosan or biodegradable polymers like poly (L-lactic acid) (PLLA), PCL and epoxy resin along with the hardener. To synthesize the nanodiamonds, A large variety of methods have been employed, such as direct synthesis at ultrahigh pressures and temperatures, electron and ion beam techniques, chemical deposition of a carbon containing vapour at high temperatures and pressures, electrochemical anodic deposition, and detonation synthesis. The bottom-up method for nano-diamond synthesis is high-pressure, high temperature (HP-HT). HP-HT technique is mainly associated with the use of thermodynamically stable conditions, which are the most favorable for obtaining the perfect diamond structure. The ND powder synthesis was conducted on multianvil HP-HT apparatus (Walker Type) at University of Allahabad. Tungsten carbide (WC) anvils of 2-4 mm truncation edge-length and MgO pressure medium (octahedron) of 10 mm edge-length were used. The starting material used was graphite powder. The sample was compressed to a desired pressure (50–60KBar) at room temperature, then heated to 1200–2000◦C for 5–30 min, and then quenched and decompressed to ambient condition. A nanocrystalline form of diamond is dominant in the temperature range from 1250 to 1400◦C, whereas at higher temperatures, diamond microcrystals are primarily formed. The synthesized samples were characterized by different experimental tools like EPMA, FTIR and XRD.ND improved the optical properties of polymers due to its interesting optical properties such as a high refractive index and the capability to strongly adsorb UV light. The efficiency of absorption of PND composite was attributed to agglomerate size, concentration of ND, and its surface functionalities. The other applications of NDs include its use as a carrier for biologically active substances, biomarkers, biosensors, high efficiency adsorbents, coatings for surgical instruments, cosmetic compositions, UV screening creams and additives for dental materials. NDs have been recently used in energy storage devices because of their high surface area, good mechanical properties, high chemical stability, and relatively high conductivity. NDs have been also applied to energy conversion fields owing to the superior electric features such as electrochemical properties, optoelectronic properties, as well as thermo-electric behaviors. Modified polymer-ND composites are applied in the manufacture of aircraft, cars, tractors and ships, chemical and petrochemical industries, production of seals, cut-off devices of various kinds, in protective and antifriction coatings. The use of nanodiamonds as active filler of polymers proved to be very efficient.

Investigations On Glyme Based Na+ Conducting Polymer Gel Electrolytes For Electrochemical Applications

Deepak Kumar[a*], Kuldeep Mishra[b]

[a]Electronics and Mechanical Engineers School (Affiliated to Gujarat Technological University),Vadodara, Gujarat-390008, India;
[b]Department of Physics and Materials Science, Jaypee University, Anoopshahr, Bulandshahr-203390, India
E-mail: deepak.kumar06@gov.in

Abstract

The dependence on fossil fuels and environmental degradation due to emission of carbon may be significantly reduced by developing low-cost, earth-abundant and environment-friendly energy/power storage systems. The Li-ion batteries perform well as compared to their counterparts. But, the lithium resources are geographically concentrated to few countries only and its price is expected to grow exponentially. The research and development on alternate cell-chemistry such as sodium and magnesium is directed to provide low-cost, sustainable energy storage systems. The development of sodium batteries may be accelerated by utilizing a high-conducting polymer gel electrolyte of superior electrochemistry. We prepare polymer gel electrolyte utilizing the tetraethylene glycol dimethyl ether (TEGDME) solvent, a polymer matrix and ion-conducting salt. Detailed investigations on conductivity, dielectric, modulus and other complimentary studies will be presented to demonstrate ion-conducting properties of the fabricated electrolytes. XRD and DSC studies will be presented in support of the structural and thermal properties. Few preliminary investigations such as open circuit voltage, discharge capacity of sodium-sulfur batteries assembled using the TEGDME based gel polymer electrolyte will be discussed.

References:

[1] M.J.S. Sayali, Deepak Kumar, K Mishra, D.K. Kanchan, Recent Advances in Electrolytes for Room-Temperature Sodium-Sulfur Batteries: A Review, Energy Storage Materials 31 (2020) 352-372.

[2] F. Gebert, J. Knott, R. Gorkin III, S-L Chou, S-X Dou, Polymer electrolytes for sodium-ion batteries, Energy Storage Materials 36 (2021) 10-30.

Advanced Electrode Materials for High Performance Electrochemical Supercapacitors with Different Electrolytes

Yogesh Kumar*

Department of Physics, ARSD College University of Delhi, New Delhi-110021, India
(*Corresponding author Email: ykumar@arsd.du.ac.in)

Abstract

In this post-modern era, energy challenges are needed to be resolved. 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, carbon materials extracted from biomass and hybrid oxide composites with conducting polymers has been studied by differential scanning calorimetry (DSC), thermo-gravimetric analysis (TGA), Raman spectroscopy and FTIR. The composites have been prepared using in-situ synthesis in the presence of oxides. As a result of chemical reactions, small agglomerates of conducting polymers with sharply defined edges of carbons have been obtained, and the composites of oxides form only a large aggregate. The specific surface area of carbon and composites is very important parameter. There are various issues related to physics at nanoscale as far as capacitors concerned.

References:

[1] V. Presser, C.R. Dennison, J. Campos, K.W. Knehr, E.C. Kumbur, Y. Gogotsi, Advanced Energy Materials (2012), 7, 895–902

[2] K. Hatzell, L. Fan, M. Beidaghi, M. Boota, E. Pomerantseva, C.E. Kumbur, Y. Gogotsi, ACS Applied Materials and Interfaces, (2014)

[3] Yogesh Kumar, G. P. Pandey, S. A. Hashmi, J. Phy. Chem. C,116, 2012, 26118-26127

[4] Yogesh Kumar, S. A. Hashmi, G. P. Pandey, Solid State Ionics, 201 (2011) 73-80

[5] Yogesh Kumar, S.A. Hashmi,G.P.Pandey, Electrochim Acta,56 (2011) 3864

Eco-friendly Polymer Electrolytes for Electrochromic Devices

Agnieszka Pawlicka

IQSC-Universidade de São Paulo, Av. Trabalhador São carlense 400, 13566-590 São Carlos-SP

Abstract

Polymers extracted from nature, i.e., from fast-growing plants or waste of plants-based production are very promising row materials to be applied as polymer electrolytes for electrochromic devices. These polymers are polysaccharides that are very well known by human beings and used as food, fibers for clothes, medicines, or cosmetics. In the last decades, it was observed that they can be also used with success in modern technology of electrochemical devices, medicine, or agriculture. This is because natural macromolecules are abundant in nature, easily extracted, biocompatible with human beings, and biodegradable, so eco-friendly. Some of these macromolecules are water-soluble and some others get this property after chemical modification. Therefore, they can be processed as membranes with elastic, transparency, and good adhesion to glass and metal properties. Their water solubility is also advantageous as this solvent can be easily recycled. Polymer solubility provides a possibility to cross-link and/or add other large or small molecules to modify these materials' properties. For example, the addition of glycerol promotes the flexibility of these membranes, and the addition of some inorganic salts, ionic liquids, dyes, clay, organic and inorganic acids lead to ionic conductivity properties. As a result, these nature-based membranes with ionic conductivity properties can be used as solid or gel polymer electrolytes in electrochemical devices such as electrochromic windows. Among different gel membranes based on natural macromolecules reported in recent years can be cited those of alginate, gellan gum, and gum Arabic, among others. These nature-based materials show ionic conductivity values that range from 10-3 to 10-5 S/cm, and when applied in electrochromic devices (ECDs) they change color under applied potential from transparent to blue or from green to yellow, depending on the ECD construction.

Towards Efficient Green H2 Production by Alkaline Water Electrolysis

Diogo M.F. Santos[a], Szilveszter G. Kéki[a], MilicaVasić[b], Milan Vranes[c], Biljana Šljukić[a,b]

a Center of Physics and Engineering of Advanced Materials, Instituto Superior Técnico, Universidade de Lisboa, Lisbon, Portugal, e-mail: biljana.paunkovic@tecnico.ulisboa.pt
b University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-16, 11158 Belgrade, Serbia
c Department of Chemistry, Biochemistry and Environmental Protection, Faculty of Science, University of Novi Sad, TrgDositejaObradovića 3, 21000 Novi Sad, Serbia

Abstract

Alkaline water electrolysis is a well-established technology for hydrogen production. If the required electricity comes from renewable energy sources (e.g., solar, wind), green hydrogen will be produced. However, global hydrogen production is still based on highly polluting steam methane reforming. Improving hydrogen (HER) and oxygen evolution reaction (OER) efficiency is essential to make electrolysis competitive with current fossil fuel-based methods. Most research has been focused on developing efficient electrocatalytic materials. Still, other approaches can decrease the activation over potential of the electrode processes. One of those is based on electrolyte additives, such as room temperature ionic liquids (RTILs). Improved HER kinetics due to RTILs addition has been previously confirmed in alkaline and acidic solutions [1,2]. RTILs can be tailor-made to increase their beneficial effect on the HER and OER kinetics. Recent studies have examined four RTILs, two commercial (3-ethyl-1-methylimidazolium chloride (C2) and 3-butyl-1-methylimidazolium chloride (C4)) and two newly tailored (3-(2-methoxyethyl)-1-methylimidazolium chloride (C1OC2), and 3-(2-ethoxyethyl)-1-methylimidazolium chloride (C2OC2)) RTILs having the same chloride anion and different alkyl chains in the methylimidazolium cation. The effect of adding small amounts (1 vol.%) of the RTILs on the HER and OER kinetics in alkaline solution (8 M KOH) is analysed. Typical electrochemical methods (e.g., voltammetry, chronoamperometry) were carried out with Pt electrodes in the 25 - 80 ºC range to calculate relevant kinetic parameters. Gas volume measurements were done in a small-scale alkaline electrolyzer to compare the gas production in 8 M KOH solution and after adding the chosen RTILs.

References:

[1] L. Amaral, J. Minkiewicz, B. Šljukić, D.M.F. Santos, C.A.C. Sequeira, M. Vraneš, S. Gadžurić, Journal of The Electrochemical Society 166, F1314 (2019).
[2] L. Amaral, J. Minkiewicz, B. Šljukić, D.M.F. Santos, C.A.C. Sequeira, M. Vraneš, S. Gadžurić, ACS Applied Energy Materials 1(9), 4731 (2018).

Lithium-sulfur batteries: where are we now?

Maria Giovanna Buonomenna

Ordine dei Chimici della Campania, Via A. Tari, 22 80138 Naples, Italy and MIUR
E-mail address: mg.buonomenna@chimici.it

Abstract

Lithium-sulfur batteries belong to the group of next generation batteries, i.e. batteries that extend their performance beyond the intrinsic limits of Li-ion batteries. The lithium-sulfur cells offer a substantial increase in gravimetric energy density, reduced costs and improved safety. However, there remain relevant challenges concerning the rate performance and cell longevity. In this presentation, after a brief overview of the current context and technical challenges for the development of lithium-sulfur batteries, advances in the knowledge of electrochemical mechanisms occurring, in exploring cathodes, separators and electrolytes will be reported.

Effective Efficiency Enhancement in Silicon Photovoltaics with Alternative ARC and Gettering

S. K. Rath*[1], R.M. Pujahari[2] and M. C. Adhikary[1] M. H. Priyadarsini

[1] Applied Physics and Ballistics, F M University, Balasore, Odisha,India[2.] ABESIT, Ghaziabad, India,
* Corresponding author E-mail: sanjit789654@gmail.com

Abstract

Silicon photovoltaics has already proven its credentials in producing commercial grade solar energy and account for almost 95% of the photovoltaic energy production. In this paper we have encountered two efficiency limiting factors. First of all we are focusing on production of a contamination free substrate by depositing the abundant metallic impurities to less harmful regions. This process is called "gettering". This article presents the design of possible routes and gettering sinks in cell architecture. Here we have discussed the method and steps involved in gettering process i.e. (release, diffuse, capture). With evolving cell fabrication techniques the potential benefits of a gettered multi crystalline silicon solar cell is summarised. In the second stage, a comparison between ZnO nano needle array and Al nanoparticles with 75nm Si_3N_4 coating as an alternative ARC is suggested. Significant photo current enhancement by supporting surface plasmon resonances to scatter light into the cells proves Al nanoparticles are impressive to produce a competent light trapping surface to improve the cell efficiency. At the other hand exceptional light trapping performance over a wide spectrum (350nm-1100nm), cost effective and elementary preparation of ZnO nano needle array made itself worth comparable.

Keywords: Gettering, Silicon Photovoltaics, Metallic impurities, Nano needle array, Surface plasmon resonance, light trapping surface

Characterization of ZnTe thin Films Prepared by Cathodic Electrodeposition as a Back Contact Buffer Layer to CdS/CdTe Solar Cells

Shivaji M Sonawane[1,2], S N Chaure[3], N B Chaure[1]

[1]Electrochemical Laboratory, Department of Physics, S P Pune University, Pune, 411007, India
[2]Department of Physics, Bharatiya Jain Sanghatana's Arts Science & Commerce College ,Pune - 412207, India.
[3]Department of Physics, College of Engineering, Pune, 411005, India.
[1]Corresponding author:n.chaure@physics.unipune.ac.in

Abstract

Zinc telluride (ZnTe), II-VI compound semiconductor is considered to be a potential candidate for applications in the field of solar cells due their appropriate optoelectronics properties. ZnTe is a p-type material with a wide and direct bandgap of 2.26eV at room temperature with electron affinity of 3.53eV.ZnTe is used as a buffer layer in the CdS/CdTe solar cell as back contact to improve performance of solar cell devices.

ZnTe thin films have been synthesized using a cathodic electrodeposition process from an acidic aqueous solution on FTO substrates. The samples were electrodeposited at -0.9V with respect to Ag/AgCl reference electrode and heat-treated at temperature 450°C for 15mins at ambient atmosphere. The samples were characterized to study the optical, structural, morphological, compositional and electrical properties by using UV-Vis-NIR spectrophotometer, X-ray diffraction (XRD), Raman spectroscopy, Field emission scanning electron microscopy, Energy dispersive spectroscopy, X-ray photoelectron spectroscopy (XPS) and Current density-Voltage (J-V) and Capacitance -Voltage measurements. The as prepared samples revealed amorphous behavior, whereas thermal heat treatment the cubic polycrystalline ZnTe samples were obtained. The energy band gap was found to be decreased ~ 5 to 7% upon heat –treatment due to the enhancement in particle size and reducing the defects/strain within the crystal lattice. The globular surface morphology with nearly uniform in grain size was obtained from FESEM images. All the samples were well compact and well adherent to the substrate. Further nearly stoichiometric ZnTe samples were obtained upon heat-treatment. The J-V measurements demonstrate the Schottky behavior of the Metal-Semiconductor contact. The Mott-Schottky plot ($1/C^2$ Vs V) exhibited the clear accumulation, inversion and depletion region. The carrier concentrations were estimated from the Mott-Schottky plot is in the order of 10^{-19} cm^{-3}, which is good conductivity suitable to make the low resistive back ohmic contact to CdTe. XPS technique confirms the presence of Zn^{2+} and Te^{2-} valence state of an elements formation during ZnTe electrodeposition.

Key-Words: Zinc Telluride, Back Contact, Thin film, buffer layer, Electrodeposition.

Structural, Optical and Electrical Properties of the ZnS and $Zn_{1-X}cd_{x}s$ Nanoparticles for Solar Cell Application

Harit Kumar Sharma[1a)], S. L. Agrawal[1b)], S. K. Pandey[1c)] and P. K. Shukla[2]

[1a,b]SSI Laboratory Department of Physics APS University Rewa (M.P.) 486003
[1c]Government Engineering College Rewa
[2] I.T.S Engineering College, Greater Noida (U.P.) - 201308
E-mail: haritsharma2@gmail.com, sla_ssi1956@rediffmail.com, skpandeygecrewa@gmail.com,
pks.vits@gmail.com,

Abstract

Present work is aimed to defect studies during the synthesis stage of $Zn_{1-x}Cd_{x}S$ semiconducting QD's prepared by a simple wet chemical precipitation method and characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), atomic force microscopy (AFM), UV-visible spectroscopy, and electrical measurements to study how the substitution of Cd^{2+} ions affect the structural, morphological, optical and electrical properties of ZnS. XRD studies confirm that all the prepared samples are in zinc-blend phase with particle size in quantum dot regime. The gradual shift of diffraction peak positions towards lower diffraction angles with increase of Cd concentration (from 0 to 0.75) indicates that the crystals are not a simple mixture of pure ZnS and CdS rather a solid solution of $Zn_{1-x}Cd_{x}S$. SEM and AFM images show microstructural information of as prepared samples with increase in particle size upon enhancing Cd^{2+}Supporting XRD result. UV-visible studies reveal that the strong absorption edge shifts towards the higher wavelength region and so the optical bandgap decreases with the increase of Cd content as a result of the crystallinity, larger grain size growth and the decreased in defect states near the bands and these turns decrease the value of Eg. Transport mechanism of the QD's is a double activation process described by Mott-Davis model showed that both electron concentration and mobility increase with increasing Cd concentration which is ascribed to the scattering of electrons by crystal defects and interfaces and the effect of a native space charge region at the near-surface region of the as prepared samples.

Structural and Ion Transport Study of CS Based Biopolymer Electrolyte Films

A. L. Saroj

Department of physics, Institute of Science, BHU, Varanasi, U. P. -221005
Email: al.saroj@bhu.ac.in

Abstract

Bio-polymers/and polymer blends are interacting materials for the preparation of polymer electrolyte films. Due to the presence of different functional groups with the side chains of biopolymer like Chitosan (CS), they easily interacts/cross-linked with the additives/polymers. Present study is basically focused on the effect of ionic liquid/salt on structural, thermal and ion transport properties of Chitosan (CS) based bio-polymeric films. The polymeric films based of CS were prepared using solution cation method. XRD results show the semicrystalline nature of CS with broad haloand it also shows that amorphousness changes significantly with the addition of ionic liquid (IL)/salt content. ATR-FTIR analysis shows the interaction/complexation between the functional groups of CS with the dopant salts/IL. Dielectric properties, Ac conductivity, ionic transference number measurement, linear sweep voltametric (LSV) measurements were carried out to understand the ion transport mechanism for prepared IL based BPE films.

Keywords: Biopolymer, ATR-FTIR, XRD, CV

Capacitance of PPy/rGo/Ni$(OH)_2$ Nanocomposite for Supercapacitor Applications

M. H. Priyadarsini*[1], M. C. Adhikary[1], R. M.Pujahari[2], S K Ratha[1]

[1]PG Department of Applied Physics and Ballistics, F. M. University, Balasore, Odisha, India
[2]ABES Institute of Technology, Ghaziabad, UP, India
* Corresponding author E-mail: mhpriyadarsini1@gmail.com

Abstract

The global energy consumption is increasing noticeable and it is predicted that the requirements of energy may be doubled by the year 2030 and 2050 respectively. Now a days conducting polymer with transition metal ions have attracted more research attention due to potential applications. Based on a conducting polymer like polyperole (PPy), graphene oxide (rGo), and Ni(OH)2 for supercapacitor applications. The morphological characterization were carried out by the Field Emission Scanning Electron Microscopy(FESEM) and Transmission Electron Microscopy (TEM) and the electrochemical performance of the nanocomposite was characterized by CV and GCD analysis. The composite showed the highest specific capacitance 97% retention over 1000 cycle.

Keyword: Polyperole, Graphene, Nanocomposite, Capacitance, TEM

Selective and Sensitive Determination of Dual Drugs on A Molecularly Imprinted Polymer/ Reduced Graphene Modified Electrode

Ritu Singh, Akriti Srivastava, Manjeet Harijan and Meenakshi Singh

Department of Chemistry, MMV
Banaras Hindu University, Varanasi-221005, INDIA
E-mail: meenakshibhu70@gmail.com

Abstract

The aim of work is to design novel molecularly imprinted polymer (MIP) matrix using 3-thiophene acetic acid (3-TAA) as monomer for simultaneous determination of more than one analyte (drug). The imprinting matrix was fabricated onto reduced graphene oxide modified glassy carbon electrode (rGO/GCE) to develop an electrochemical sensing platform. The analytes used here are ethionamide and antipyrine being used as model templates during imprinting. 3-TAA was electropolymerized using cyclic voltammetry technique in presence of templates onto rGO/GCE to form imprinted polymer. The MIP film formation was confirmed using electrochemical techniques and AFM analysis. Results showed the successful imprinting of templates and formation of imprinted cavities were achieved on removal of the analytes from the polymeric matrix using suitable extracting solvents. Analysis of analytes were performed using differential pulse voltammetry as electrochemical technique. The response increased linearly in range of 0.05 µM to 0.6 µM with LOD of 0.11 µM for antipyrine and 0.03 µM to 1.2 µM with a detection limit of 0.15 µM for ethionamide, respectively. The developed MIP sensor was found to be highly sensitive and selective for imprinted analyte molecules.

Quantum Chemical Calculations on Molecules with Donor-Π-Acceptor Structures for Efficient Organic Field Effect Transistor

Ankit Kargeti[1], Shamoon Ahmad Siddiqui[2,3], Tabish Rasheed[1]

[1]School of Engineering and Technology, BML Munjal University, Gurugram, Haryana, India 122413.
[2] Promising Centre for Sensors and Electronic Devices, Najran University, Najran, KSA 11001.
[3] Department of Physics, Najran University, Najran, KSA 11001.

Abstract

Novel organic compounds for possible use in organic field effect transistors (OFETs) have been widely researched in recent times. Polythiophene[1] was the first organic compound to be used for development of OFET in 1986. OFETs with *p*-type semiconductor properties have been found to be most suitable for designing of devices, since, stability of such compounds is higher as compared to *n*-type semiconducting compounds. In this paper, two molecular structures(naphthalene-pyrrole-propanoic acid and naphthalene-pyrrole-pyridine) have been designed based on the donor-π-acceptor architecture. Both structures were optimized using density functional theory (DFT) at B3LYP/6-31+G (d,p) theory level. These structures were also checked to confirm whether they correspond to global minima on potential energy surface (PES) through frequency calculation in the *Gaussian 16W* software package. Thorough analysis of calculated parameters such as hole reorganization energy (λ_h), electron reorganization energy (λ_e), ionization potential (vertical and adiabatic) and electron affinity (vertical and adiabatic), has been done to investigate charge transport properties. In both the designed systems, λ_h values were found to be smaller as compared to λ_e values. Hence, it may be inferred that our designed molecules have holes as majority charge carriers and can be utilized as p-type semiconductors. Behavior of both designed molecules under electric field was also checked to determine their feasibility for use as conducting channel in OFET.

Keywords: donor-π-acceptor, OFET, DFT, reorganization energy.

References:

1. A. Tsumura, H. Koezuka, T. Ando, Applied Physics Letters. 49 (1986) 1210–1212

Investigation for Structural, Electronic and Optical Characterization of Lithium-Based Chalcopyrite Semiconductors by Using Density Functional Theory

Jyoti Kumari[1*], Banwari Lal Choudhary[1] and Ajay Singh Verma

[1]Department of Physics, Banasthali Vidyapith, Rajasthan (India)304022
[2]Department of Natural and Applied Sciences, Glocal University, Saharanpur (India) 247232
*Corresponding author: Jyotidhankhar284@gmail.com

Abstract

The ab-initio calculations have been executed by the authors for structural, electronic and optical characterization of $LiAlTe_2$, $LiGaTe_2$ and $LiInTe_2$ chalcopyrite structured semiconductors these calculations are grounded on the principle of density functional theory (DFT) employed into the WIEN2K simulation code. Authors used full potential linearized augmented plane wave (FP-LAPW) for the investigation of mentioned properties. The computed lattice constants oscillating from a = 6.257 Å to 6.450 Å and c = 12.044 Å to 12.256 Å for $LiXTe_2$ (X=Al, Ga and In) also these values consistent with experimentally existed lattice constants. From the study of electronic band-gap it confirms that these three compounds are semiconductors with direct band-gaps. The results of optical properties confirm that these chalcopyrite semiconductors can be the fortunate compounds for the solar cell applications.

Keywords: WIEN2K, Chalcopyrite, Semiconductors, Band-gap and DFT.

Review on electrochemical kinetics of Carbon Dots

Vishal Rimal*, P.K. Srivastava

Department of Chemistry,
Birla Institute of Technology, Mesra, Ranchi, India, 835215

Abstract:

Carbon Dots (CDs) are zero-dimensional carbon nanomaterials that can be doped with N, S, P, and B heteroatoms to boost their properties. CDs have attracted significant interest over the past decade due to their outstanding physicochemical properties, which are complemented by their low cost, green chemistry, and excellent stability. The combination of CDs with traditional electrochemical materials has been found to alter the kinetics of electrochemical reactions. This review aims to underline the notable results on the electrochemical kinetics of CDs. The advances in this domain would promote the development of fuel cells, water electrolysis, and rechargeable metal-air batteries and pave new directions on the applicability of CDs.

Keywords: Carbon Dots, electrochemistry, kinetics

Functional Biochar Derived from *Desmostachyabipinnata* for the Application in Energy Storage/Conversion Devices

Meenal Gupta[*1], **Smriti Mehrotra**[2], **Kouao Dujearic-Stephane**[1], **Ashwani Kumar**[3], **Pushpa Singh**[4], **Abhilasha Singh Mathuriya**[2*],**Yogesh Kumar**[*5]

[1]Department of Physics, SBSR, Sharda University, Greater Noida 201 310, India
[2]Bio-POSITIVE, Department of Life Sciences, SBSR, Sharda University, Greater Noida 201 310, India
[3]Nanoscience Laboratory, IIC, Indian Institute of Technology, Roorkee 247667, India
[4]Department of Zoology, SSN College, University of Delhi, New Delhi-110036, India
[5]Department of Physics, ARSD College, University of Delhi, New Delhi-110021, India

Abstract

In the present work, biochar is synthesized from grass *Desmostachyabipinnata* using simple carbonization at 800°C under nitrogen atmosphere without using any activating agent. The morphology, crystalline state, vibrational surface area and porous study and thermal properties of the biochar are investigated using Field Emission Scanning Electron Microscope (FE-SEM),X-Ray diffraction analysis (XRD), Raman, Fourier Transform Infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), Brunauer–Emmett–Teller (BET) and Thermogravimetric analysis/Derivative Thermogravimetry (TGA/DTG). The oxygen containing surface functional groups in biochar are assessed. This biochar material is used to develop electrode material in supercapacitors. A comparative study of the electrochemical properties of the fabricated supercapacitor is conducted using cyclic voltammetry (CV) studies and electrochemical impedance spectroscopy (EIS) with 1-ethyl-3-methylimidazolium thiocyanate (EMImSCN) ionic liquid and 1M H_2SO_4 electrolytes. The prepared electrodes exhibited enhanced capacitive performance, ~ 26 F/g for 1M H_2SO_4 electrolyte as compared to ~ 22 F/g for EMImSCN ionic liquid.

Keywords: Biochar, *Desmostachyabipinnata* grass, BET analysis, ionic liquid, porous electrodes

Heating Effect, UV Radiation and Trap Depth Parameters of Rare Earth Doped Yttrium Oxide for Dosimetry Applications

Manmeet Kaur[1] **and Prabhjot Singh**[2]

[1]Dept of Applied Physics, Shri Shankaracharya Technical Campus, Bhilai, Chhattisgarh, India, 490020
[2]Bharti College of Engineering & Technology, Durg, Chhattisgarh, India, 491001
Corresponding authors: manmeet.bhuie@gmail.com

Abstract

Thermoluminescence Characteristics of Y_2O_3:Er^{3+} nanophosphors exposed to UV radiations have been investigated. Combustion Synthesis method was employed to synthesis the nanophosphors. The crystal structures of the prepared phosphors were identified from XRD studies and revealed that the synthesized particles have a pure body centered cubic Y_2O_3 structure with space group Ia_3(206). TEM confirms the spherical shape of the particles and results were in close agreement with the XRD. Thermoluminescence studies were carried out after irradiating the phosphors by UV radiation. The trapping parameters (μ, E, s) were calculated from Chen's glow peak shape method and Trap depth associated with different trap levels was calculated from thermoluminescence data using various glow curve analysis techniques. TL Glow curve was also fitted in CGCD (computerized glow curve deconvolution) techniques using origin 8.0 software and were discussed in detail for their possible usage in dosimetry applications

Keywords: Nanophosphors, X ray diffraction, Combustion Synthesis, Thermoluminescence, CGCD.

Fast and Stable Electrolyte Scandium Co-Doped Barium Cerate

Bibek Kumar Sonu, Ela Rout[1]

Department of Physics, Birla Institute of Technology, Mesra, Ranchi, India – 835215
[1*]Correspondence to E-mail: elasinha@gmail.com

Abstract

Proton conducting barium cerate ceramics co-substituted with scandium and zirconium$BaCe_{0.8-x}Zr_{0.2}Sc_xO_3$ (x = 0, 0.05, 0.10, 0.15, 0.20) has been prepared by the traditional solid-state reaction process. The X-ray diffraction patterns confirmed the single-phase orthorhombic symmetry of the synthesized samples. The thermal stability of the ceramics has been checked by thermogravimetric analysis (TGA). TGA of dry and pre-hydrated (pH_2O (g) ≈ 0.03 atm and 1.0 atm) samples revealed that all the samples are stable up to a temperature of 800 °C. However, the samples smoked at a higher partial pressure of water are less stable. The crystalline phase of the studied compositions before and after TGA was measured with the Raman study, confirming that most of the parent phases exist or remain stable even after the treatment of samples at higher vapor pressure. Thermal stability progressively improved with increasing Sc-substitution. The TGA results that are consistent with the Raman studies proved the sample with x = 0.20 is the most stable amongst the studied compositions. Complex impedance spectroscopy (CIS) readings clearly demonstrated the impact of bulk and grain boundary on the total resistance of the compounds with different scandium contents. Comparing the conductivity under dry and wet atmospheres suggests that some additional charged species participate in the conduction mechanism under the wet environment. These are ascribed to the protonic defects, developing into barium cerate via intrinsic oxygen vacancies because of trivalent (Sc) doping at cerium site.

Keywords: Proton conduction, Ceramics, Raman spectroscopy, Impedance study, Thermogravimetric analysis.

Synthesis of H_2O_2 Refluxed $LaFeo_3$ Loaded as Filler Inpoly (Vinylidene Fluoride) for High Energy Density Storage Applications

Vishwa Pratap Singh[1,2], Chandra Bhal Singh[2], Satyendra Kumar Satyarthi[1,2], Dinesh Kumar[2], Akhilesh Kumar Singh[2]

[1]Department of Ceramic Engineering, Indian Institute of Technology (BHU), Varanasi, India[2]School of Material Science and Technology, Indian Institute of Technology (BHU), Varanasi, India
*Email: vishwapsingh.rs.cer17@itbhu.ac.in

Abstract

In this work, the solution cast method is used for the preparation of poly (vinylidene fluoride) (PVDF)/ refluxed $LaFeO_3$ composite film. The refluxed $LaFeO_3$ is used as filler in the PVDF film for the improvement in the dielectric and ferroelectric properties. The H_2O_2 refluxing improves the interfacial interaction between the filler and PVDF matrix. The polar phase increment has been seen in refluxed $LaFeO_3$ loaded PVDF film by the interfacial interaction due to -OH bond. The structural and morphological analysis has been done for the phase identification with the help of XRD, FTIR and HR-SEM. XRD and FTIR analysis confirmed the formation of polar phases (β, γ-phase) in dominance with non-polar phase (α-phase).The dielectric constant and ferroelectric properties have been improved with the help of loaded filler. The ferroelectric hysteresis loop is recorded to study the ferroelectricity in the H_2O_2 refluxed $LaFeO_3$/PVDF composite film.

Keywords: Dielectric constant, poly (vinylidene fluoride), Energy density.

Simple and Rapid Ecofriendly Synthesis of NiO/RGO Nanocomposites using Guava Leaf Extract and their Physicochemical Characterization

Priyanka Lamba[1,7], Parul Singh[2], Pankaj Singh[1], Ashwani Kumar[3], Pushpa Singh[4], Bharti[5], Yogesh Kumar[6*], Meenal Gupta[7*]

[1]Department of Physics, Deshbandhu College, University of Delhi, Kalkaji, New Delhi-110019, India
[2]Department of Chemistry, Deshbandhu College, University of Delhi, Kalkaji, New Delhi-110019, India
[3]Nanoscience Laboratory, I. I. T., Indian Institute of Technology, Roorkee 247667, India
[4]Department of Zoology, SSN College, University of Delhi, 110 036 New Delhi, India
[5]Shivaji College, University of Delhi, Mahatma Gandhi Marg, Shivaji Enclave, Raja Garden, Delhi 110027, India
[6]Department of Physics, A R S D College, University of Delhi, New Delhi-110021, India
[7]Department of Physics, School of Basic Sciences and Research, Sharda University, Greater Noida - 201310, India

Abstract

In the present communication eco-friendly synthesis of Nickel oxide/reduced graphene oxide (NiO/RGO) nanocomposites is reported. NiO/RGO nanocomposites were synthesized via green route. Guava leaves extract is used and reducing agent. The morphological and structural properties of synthesized samples were analyzed using Ultraviolet Visible Spectrometer (UV-VIS), X-Ray powder diffraction (XRD), Scanning electron microscopy (SEM), Raman Spectroscopy, Fourier transforms infrared spectroscopy (FTIR), X-Ray photoelectron spectroscopy (XPS) and Differential thermal analysis (DTA). It is evident from results that NiO nanoparticles successfully incorporated into RGO sheets and form a composite structure. Moreover, the synthesized composites might find application in catalysis and energy storage devices.

Keywords: Graphene Oxide**,** Nanocomposites**,** Phytoextract, Green Route

Structural, Electronic and Mechanical Properties of Hybrid h-BN/Graphene 2D layers: Density Functional Approach

B Keshav Rao

Department of Applied Physics
Shri Shankaracharya Technical Campus, Bhilai (Chhattisgarh) India
E-mail: b.keshav26@gmail.com

Abstract

The first principle calculations based on density functional theory are performed. In the simulation, a single unit of a 2D-hybrid atomic chain 6-BNGR, in which 6-BN molecules of an atomic chain comprised of 16 BN molecules are replaced by 6-carbon pairs, and transformed into 6-BNGR-2U, 6-BNGR-3U & 6-BNGR-4U 2D-hybrid atomic layers, where GR and U represent to a graphene and a single unit, respectively. The bond length analysis indicates to a strong interaction in hybrids without vacancy. The total density of states and the band diagrams exhibit the metallic nature of all hybrids, during the transition from a 2U hybrid to 4U hybrid, upward shifting is found in the bottom of the density of states. In the presence of external electric field applied normal to the length of layers, higher shifting in the density of states is observed at 9 V/Å. The stress strain analysis exhibits 6-BNGR-2U and 6-BNGR-4U-2, where 2 represents 2-vacancies, has higher strength during expansion and in compression along y-axis, 6-BNGR-4U-2 has higher strength along z-axis. The strain along z-axis exhibits a significant shifting in the bottom of the density of states. Hence, due to shifting in the bottom of the density of states, hybrids respond faster in the electronic properties which can be applied in the metallic device applications.

Keywords: Density functional theory; SIESTA; Hybrid structure; Density of states.

Synthesis and Characterization of Aryl Substituted 4- Thiazolidino A,B – Unsaturated Ketones and Dimethyl Amino Methylene Ketones and their Biological Activity

Dhirendra Kumar

Department Of Chemistry
Shri Venkteshwara University, Gajraula, Distt.- Amroha (U.P.)

Abstract

The biggest category of organic chemicals is heterocyclic. For a wide range of industrial, medical and traditional applications they are essential. The integration of new Heterocyclics is growing need for innovative and efficient methods. Create eco-friendly and competitive solutions combined with green technology is an essential synthetic network test. The heterocyclic delegated compounds are possibly the large and diverse organic category. Each carbocyclic compound with its structure and utility, little consideration maybe transform into a heterocyclic range of analogues at the fundamental level by replacing at least one of the least carbon molecules with an alternative component regardless of whether we limit our thinking to oxygen nitrogen and sulphur, there are particular alterations and combinations. Heterocyclic chemistry is an endless source of new molecules and almost unlimited carbon hydrogen heteroatomic combinations maybe designed.

These make it very easy to understand the enormous dispersion and significance of heterocyclic substances that are composites with the most diverse physical synthetic and organic characteristic. A study of the preferred natural compounds shows an impressive preference in the formation not of carbon bonds but of carbon heteroatom bonds, serenely not a surprise because carbon dioxide is the begin material for nature and most of the reactions occur in water. Condensation polymers of the tiny subunit stitched together by a carbon heteroatom link include nucleic acids proteins and poly saccharides.

Heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. This especially true for five member ring heterocyclic compounds which serve as the core compounds of a large number of substances that possess a wide range of interesting biological actives. Among them oxygen sulphur and nitrogen containing five membered heterocyclic compounds have mentioned the interest of researchers through decades of historical development of organic synthesis. The grounds of the interest were there biological activities and unique structure that lead to several applications in different areas pharmaceutical and agrichemical research or more recently in material sciences.

Different Derivatives of aryl substituted 4 –thiazolidino α,β – unsaturated ketones and dimethyl amino methylene ketones were synthesized and had been confirmed by IR,^{1}HNMR and Mass spectra. They have found to possess severity of the rapeutic profile including anti-bacterial, anti-fungal, anti-microbial and anti-inflammatory activity.

Impact of the Bath Temperature on CdTe Thin Films Prepared by Electrochemical Technique

Aparna Ukarande[1], S.Chaure[2]and N.B.Chaure[1],

[1]Electrochemical Laboratory, Department of Physics, Savitribai Phule Pune University, 411007,
[2] Department of Physics, College of Engineering, Pune, 411005,
Corresponding author: n.chaure@physics.unipune.ac.in

Abstract

Cadmium telluride (CdTe) thin films have been prepared by using potentiostatic electrodeposition technique on to FTO coated glass substrates from an aqueous solution. The cadmium sulphates ($CdSO_4$), tellurium oxide (TeO_2) were used as the source of Cd and Te ions. Citric acid ($C_6H_8O_7$) was used as complexing agent to enhance the conductivity of the bath and to obtain the stoichiometric layers at desired potentials. A conventional three electrode geometry was employed for the deposition of CdTe layers. The deposition potential was optimized with help of cyclic voltammetry experiment. CdTe layers were electrodeposited at -0.7V. The effect of bath temperature on the structural, optical and morphology properties was studied. The deposited samples were annealed in ambient condition at temperature 450˚C for 20 min. The reflection peaks exhibited around 23°, 39° and 46° are corresponds to (111), (220) and (311) planes of cubic CdTe. The degree of crystallinity was found to be enhanced upon heat treatment. Te metallic peak was observed in an annealed sample for the sample deposited at 70°C, which is probably due to the higher kinetic energy gained by the Te ions. Upon annealing the sample deposited at 50°C was without metallic Te. From Raman analysis, it showed that the longitudinal optical vibration mode symmetry, enhancement in crystallinity, and improvement in the material quality of CdTe thin films. The estimated energy band gap value for annealed sample was ~1.45 eV. Uniform, dense and compact morphology were observed from SEM analysis.

Keywords: Cadmium telluride (CdTe), Electrodeposition, Thin films, Characterization.

References:

1. Jun Wang, Shurong Liu et. al. Journal of Alloys and Compounds, 18, 8388 (2018).
2. I. M. Dharmadasa1, O. K. Echendu, et. al., J Mater Sci: Mater Electron 28, 2343–2352, (2017).
3. F. de Moure-Flores, J. G. Quiñones-Galván, et. al., Journal of Applied Physics 112, 113110 (2012)

Analytical Analysis of Concentration of Charge Carriers in Polymer Electrolytes through Different Models

Amit Saxena[1] **and Bhaskar Bhattacharya[2]**

[1] Department of Physics, SVIS, Shri Vaishnav Vidyapeeth Vishwavidyalaya, Indore, M.P. INDIA

[2] Department of Physics, MMV, Banaras Hindu University, Varanasi, U.P. INDIA

Abstract

The development of solid polymer electrolytes with high ionic conductivity and good chemical and mechanical stability for application in various electrochemical devices has been an important area of research in the past few decades[1]. For the better performance of the electrochemical devices, the compatibility between the electrodes and electrolytes of the system is the foremost requirement. In addition to this, the ion conductivity of the electrolytes is an important parameter. Understanding the mechanism of changes in ionic conductivity with different concentrations of salt and dispersoid is very crucial[2]. In the present work different theoretical models, like the Rice-Roth model, Trukhan model and Schutt and Gerdes Model, have been used to calculate and analyse the concentration of charge carriers[3]. For this, all the parameters of the models are being taken from Impedance spectroscopy data. Trukhan model is a direct and simple method for evaluating the exact value of the diffusion coefficient. The diffusion coefficient of PEO-NaI based electrolyte is calculated from the dielectric tangent loss and further used for analyzing the concentration of charge carrier and ion mobility. Similarly, two more theoretical models, Rice-Roth and Schutt and Gerdes Model were used to confirming the value of the number of charge carriers and further all the results were compared with each other for the conclusion[4].

Keywords: Polymer Electrolytes, Concentration of Charge Carriers, Rice-Roth model, Trukhan Model, Schutt and Gerdes Model.

References:

[1] A. S. Abd-El-Aziz *et al.*, “The Next 100 Years of Polymer Science,” *Macromol. Chem. Phys.*, vol. 221, no. 16, pp. 1–22, 2020, doi: 10.1002/macp.202000216.

[2] R. Singh, P. K. Singh, V. Singh, and B. Bhattacharya, “Quantitative analysis of ion transport mechanism in biopolymer electrolyte,” *Opt. Laser Technol.*, vol. 113, no. May, pp. 303–309, 2019, doi: 10.1016/j.optlastec.2018.12.036.

[3] T. M. W. J. Bandara, L. A. DeSilva, L. B. E. Gunasekara, S. Dehipawala, and B. E. Mellander, “Determination of charge carrier transport parameters in a polymer electrolyte intended for Li-ion batteries using electrochemical impedance analysis,” *J. Solid State Electrochem.*, vol. 24, no. 5, pp. 1207–1216, 2020, doi: 10.1007/s10008-020-04604-3.

[4] S. Dutta, “Review on Solar Hydrogen: Its Prospects and Limitations,” *Energy and Fuels*, vol. 35, no. 15. American Chemical Society, pp. 11613–11639, Aug. 05, 2021, doi: 10.1021/acs.energyfuels.1c00823.

AC Conductivity and Ion Dynamics Behavior Study of PVA Based Polymer Electrolyte Films

Pooja Rawat and A. L. Saroj

Department of Physics, Institute of Science, Banaras Hindu University, Varanasi-221005, India
*****E-mail: al.saroj@bhu.ac.in

Abstract

Impedance spectroscopy (IS) is a very versatile tool to measure the electrical properties of dielectric/amorphous materials and their interfaces. It is used to study the ion dynamics behaviour, dielectric properties and electric modulus of the ion/electron conducting solid polymer electrolytes by using frequency dependent phase and impedance data. The solid polymer electrolyte (SPE) films based on polyvinyl alcohol (PVA)-lithium tetraflouroborate ($LiBF_4$) were prepared by using conventional solution casting method. Prepared SPE films were characterized using AC impedance spectroscopic technique. The frequency dependent conductivity, dielectric properties and molecular dynamics were analyzed. Scaling of ac conductivity with respect to salt concentrations was performed for understanding the ion transport mechanism in the SPE films.

Keywords: Polymer electrolytes, AC conductivity, Dielectric properties, Scaling

Comparative Study of Physical Properties of Cold-Sintered $CuPbBr_3$ and $CuPbI_3$Perovskite for Solar Cell Applications

Prem C. Bharti*, Priyanka A. Jha, Pardeep K. Jha and Prabhakar Singh*

Department of Physics, Indian Institute of Technology (BHU) Varanasi-221005, India
*Corresponding authors: premchandrab.rs.phy17@itbhu.ac.in, psingh.app@iitbhu.ac.in

Abstract

The perovskite halides have attracted the Solar cell researchers' community on the verge of replacement of Silicon solar cells. Copper lead bromide ($CuPbBr_3$) and Copper lead Iodide ($CuPbI_3$) are the inorganic perovskite materials known for the suitability as light absorbing materials for solar cell applications. In the present work, $CuPbBr_3$ and $CuPbI_3$ are synthesized through cold sintering technique in ambient atmosphere. The XRD diffractograms revealed the single phase formation with cubic phase and hexagonal phase for the respective materials which is also verified through reported results. The thermo-gravimetric studies revealed the thermodynamical stability of the sample formed at room temperature. The band gaps 2.87eV and 2.32eV are estimated using UV-visible absorbance spectrum for $CuPbBr_3$ and $CuPbI_3$, respectively. The photo-degradation of both materials are analyzed through I-V measurement in 1.5AM-G solar light through solar simulator.

Keywords: Perovskite Halides, cold-sintering and Photo-degradation.

Synthesis, Characterization and Energy Storage Application of Carbon/Graphene Aerogel

Sweta Singh[1*]

[1]Department of Physics, Mahatma Gandhi Central University, Motihari-845401, Bihar
*E-mail: swetaphysics@mgcub.ac.in

Abstract

Here we report the synthesis and characterization of carbon/graphene aerogel and its application as hydrogen storage/EMI shielding material. The synthesis parameters adapted for carbon aerogel led to the formation of preponderance of submicro-pores. Structural and microstructural characteristics of these carbon aerogels (CA) have been investigated through XRD, SEM, TEM, nitrogen adsorption and Raman spectroscopic techniques. The hydrogen storage characteristics of as synthesized carbon aerogels have been investigated by monitoring the hydrogen ad/desorption curves. At room temperature and at pressure upto 22 atm the CA has hydrogen storage capacity of 0.40 wt.% and under the same pressure but at liquid nitrogen temperature CA has hydrogen storage capacity of 5.65 wt.% .However, graphene aerogel (GA) is one of a new exotic form of graphene nanosheet, which shows improved shielding features as compared to its pristine counterpart. The structural and microstructural characteristics of this new indigenous 3D sponge like graphene aerogel architecture have been probed by SEM, TEM, XRD and Raman. The high surface area and better porosity improve the EMI shielding effectiveness of GA. This engineered GA exhibits enhanced shielding effectiveness (20.0 dB at 0.20 g in a frequency region of 12.4 to 18.0 GHz) as compared to the conventional GO. Thus, the result of the EMI shielding of GA offers a new ingenious nanostructure which can be used as an EMI pollutant quencher for next-generation EMI shielding devices.

Keywords: Carbon aerogel, Graphene aerogel, Ultralight, hydrogen storage, EMI Shielding.

Graphitic Carbon Nitride Based Heterojunction nanocomposite for Degradation of Organic Dyes

Monika Vikal[a], Shachi Shah[a], Yogesh Kumar[b]*

[a]School of Sciences, Indira Gandhi National Open University, New Delhi-110068, India.
[b]Department of Physics, ARSD College, University of Delhi, New Delhi - 110021, India
*Corresponding authors: Yogesh Kumar,
E-mail: ykb.ssi@gmail.com, Tel.: +919999254014,

Abstract

In this work, the graphitic carbon nitride (g-C_3N_4) is synthesized using calcination of melamine in muffle furnace and metal complex containing metals Na, Fe, Ti is synthesized separately. The heterojunction nanocomposite is prepared by physical method mixing of g-C_3N_4 and metal complex. The nanocomposites were prepared in 10 wt% and 30 wt% composition of metal complex. The prepared nanocomposites are characterized using FTIR, XRD, SEM, TEM and UV-visible spectrophotometer. The energy band gap of nanoparticles are measured using Tauc plot and it is found that the energy band gap decreases from 2.53 eV for g-C_3N_4 to 2.0 eV for heterojunction nanocomposites. The nanocomposites degraded the Rhodamine (RhB) dye in less than 5 minutes and showed first order kinetics. The synthesized nanocomposites degraded both RhB and methylene Blue dye successfully.

Future Prospects of Biopolymer- Ionic Liquid Polymer Electrolyte

Subhrajit Konwar, Pramod Kumar Singh

Center of Excellence on Solar Cells and Renewable Energy, Department of Physics, School of Basic Science and Research, Sharda University, G. Noida, 201306, India
E-mail: subhrajitkonwar@gmail.com (SK); pramodkumar.singh@sharda.ac.in (PKS)

Abstract

With the increase in demand of clean and green energy, the chase in the development of bio degradable, nontoxic, ecosystem friendly materials has gain tremendous interest. In the past decades the researchers were mainly focus on the development of the new technology compromising the sustainability of the ecosystem. But looking at the present scenario different standard has been set for every technology to control the level of pollution and pollutant. Energy storage devices are the hot tropics of the present and also of the future. Most electrochemical devices comprises with electrodes and electrolyte. Polymer electrolyte already proposed as novel alternative for liquid electrolyte. Biopolymer electrolyte has disadvantage of low ionic conductivity. Low viscosity ionic liquid (IL) is proposed as novel dopants which enhances conductivity and also act as plasticizer which reduces crystallinity and enhances amorphous nature. This paper deals the importance of low viscosity IL as dispersoid. The electrical, structural and photoelectrochemical device performance are also going to describe in detail.

Keywords: Bio-Polymer, Ionic Liquid, Electrolyte, Conductivity

Structural and Bandgap Studies of $Cs(Sn_{1/2}Pb_{1/2})Br_3$

Swarnima Singh[#]**, Prabhakar Singh***

Department of Physics, Indian Institute of Technology (Banaras Hindu University), Varanasi 221005, India
Corresponding authors: swarnimasingh.rs.phy19@itbhu.ac.in[#], psingh.app@iitbhu.ac.in*

Abstract

Owing to the high toxicity of Pb based perovskite, Sn is employed to partially replace Pb with an aim of gaining environmentally-friendly optoelectronic devices with tunable bandgap. $Cs(Sn_{1/2}Pb_{1/2})Br_3$ was synthesized by the cold sintering technique. The X-ray diffraction affirms that the structure of synthesized $Cs(Sn_{1/2}Pb_{1/2})Br_3$ is orthorhombic. UV-Vis spectroscopy of the sample was done. Taucs plot gives the bandgap of 1.83 eV. Current -Voltage (I-V) characterization is also done in both the modes, in dark and in the presence of light. Studies suggest there is almost no change in the trap density in the AM 1.5 G Sun light however small increment in the current is observed.

Keywords: Tunable bandgap, Tauc plot, photoelectronic device, $Cs(Sn_{1/2}Pb_{1/2})Br_3$

Role of Natural Dye in Photovoltaic Performance of Dye Sensitized Solar Cell

Varsha Yadav[1, 2a], Yashaswi Soni[1], Chandra Mohan Singh Negi[1], Saral Kumar Gupta[1] and Upendra Kumar[3,]

[1]Department of Physical Sciences, Banasthali Vidyapith, Banasthali, 304022, INDIA
[2]School of Applied Science, Shri Venketashwar University, Gajraula (Amroha), 244221, U.P.INDIA
[3]Department of Applied Sciences, Indian Institute of Information Technology (IIIT) Allahabad, Prayagraj-211015, U.P. INDIA
*Corresponding author: [a]varshayadav616@gmail.com

Abstract:

Investigating cost-effective alternatives to organic dyes for use in dye-sensitized solar cells (DSSC) could help to lower the overall cost of the devices. This manuscript deals with optical and structural properties of novel natural dye extracted from harda fruit. The optical absorbance and emission of natural dye has been studied using UV-Vis. Spectroscopy and photoluminescence. GC-MS and FTIR analysis allow us to identify the various chemical compounds and functional groups present in the dyes, respectively. The DSSC has been fabricated using natural dye as photo-sensitizer and studied their photovoltaic performance. The power conversion efficiency (PCE) for DSSC has been achieved up to 2.7%. Although the use of natural dye in DSSC improved the better short-circuit current density (Jsc) and open-circuit voltage (Voc). Understanding these fundamental properties of natural dye could pave the way for the development of natural dyes based solar cells.

Keywords: Dye sensitized solar cells, Natural Dye, Power conversion efficiency, Anthraquinone Group.

References:

1. B. O.Regan et al., Nature, 1991, vol.353, pg. 737.
2. V Yadav et al., East Eur. J. Phys.3, 129-133, 2020.
3. M. Tripathi et al., Ionics, 2013, vol. 19, pp. 1179.
4. Y. Li et al., International journal of electrochemical science, 2013, vol. 8, pp. 1237.
5. V Yadav et al., Optical Materials, 109, 110306(1-7), 2020.

Structural and Photo-conduction studies of NiO as a Hole Transport Material for Perovskite Solar Cells

Ashish K. Ranjan[*], **Prabhakar Singh**[*]

Department of Physics, Indian Institute of Technology (Banaras Hindu University), Varanasi 221005, India
*Corresponding author:ashish.kumarranjan.rs.phy18@iitbhu.ac.in,psingh.app@iitbhu.ac.in

Abstract

Perovskite solar cells has made a remarkable progress in a very short time in photovoltaic technology. NiO is one of the inorganic hole transport materials, synthesized by using the conventional solid-state reaction route. In this work, the X-ray diffractogram affirms that synthesized NiO exhibits rhombohedral structure which was further confirmed by Rietveld Refinement. I-V plot confirms the photoconductive behaviour of NiO and a very small area of hysteresis also has been observed in AM 1.5G Sun light.

Keywords: Hole Transport Materials, Perovskite Halides, Solar Cell, Nickel Oxide, Photo-conduction

Impact of In-Situ Formed Silica Nanospheres on Physicochemical and Ionic Transport Properties of PEO-Based Hybrid Electrolytes

Sujeet Kumar Chaurasia

Centre for Nano-science and Technology, Prof. Rajendra Singh (Rajju Bhaiya) Institute, V.B.S. Purvanchal University, Jaunpur, UP-222003, India
Email of corresponding author: sujeetchaurasia@gmail.com

Abstract

In this present investigation flexible organic-inorganic hybrid electrolytes (OIHs) are prepared by incorporating inorganic silica nanoparticles (SiO_2) to the organic polymer PEO backbone via in-situ sol-gel method. The synthesized OIHs consisting of 20 wt.% of LiTf gave ionic conductivity of ~1.24 x 10^{-6} S/cm at room temperature (~30^{o}C) with lithium transference number (t_{Li+}) ~0.39. ATR-IR spectroscopic analysis confirmed the intermolecular interaction of the salt's cation (Li^+) with the polymer (PEO) backbone and/or SiO_2 matrix as well as formation of Si-O-Si skeleton framework structure within the hybrid matrix. XRD/DSC results showed that amorphicity of OIHs increases with increasing content of salt LiTf in the hybrid matrix which, in turn, responsible for enhancing the conductivity of the membranes due to increase in flexibility of the polymeric backbone. TEM images showed the appearance of silica nanospheres of size ~20 nm within the PEO-LiTf electrolyte matrix while the FESEM analysis confirmed the layered morphologies. The linear sweep voltammetry (LSV) for the highest conducting hybrid electrolyte with cell configuration SS/OIHs/Li showed electrochemical stability window of 5.2 V which is sufficient voltage range for their use in solid state Li-ion batteries and other electrochemical devices.

Keywords: Hybrid electrolyte, Ionic transport, Surface morphology, Thermal stability

Development of Porous Carbon from Polyvinyl Chloride (PVC) and Its Application in Supercapacitor

Pawan Singh Dhapola[a,b]*, Pramod K. Singh[a], Nanda Gopal Sahoo[b]*

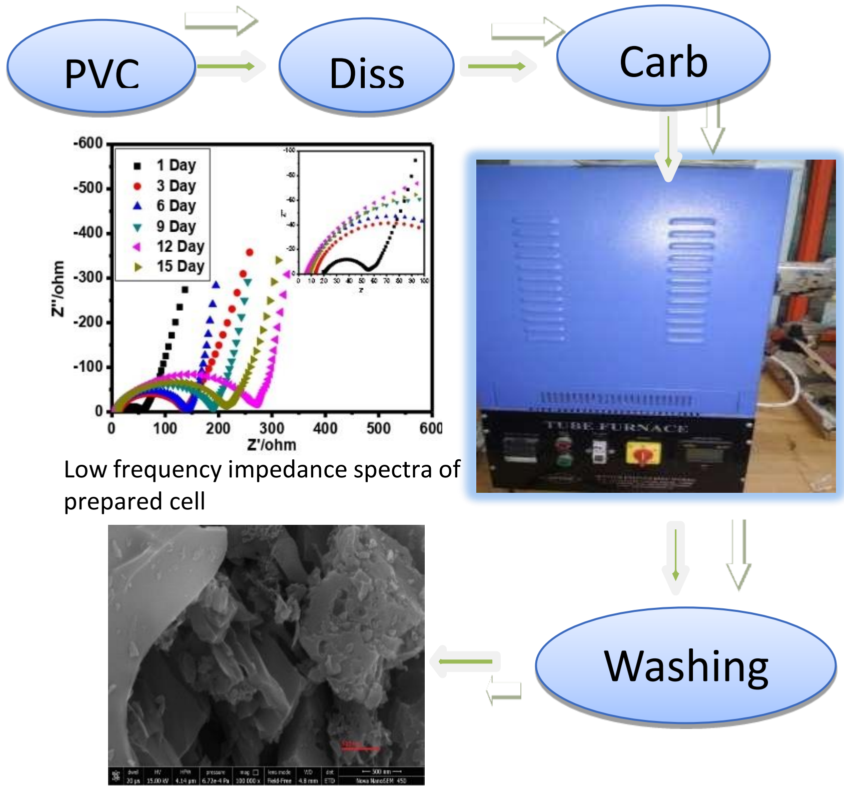
[a]Center of Excellence on Solar Cells & Renewable Energy, School of Basic Sciences and Research, Sharda University, Greater Noida.
[b]Professor Rajendra Singh Nanosciene and Nanotechnology Centre, Department of Chemistry, DSB Campus, Kumaun University, Nainital, Uttarakhand.

*Corresponding Author: dhapolapawan@gmail.com (PSD), ngsahoo@yahoo.co.in (NGS)

Abstract

In this work we have focused towards the laboratory scale production of activated carbon synthesized from PVC with $CoCl_2$ and H_3PO_4, which is cheaper and having good yield source material. We have successfully developed a supercapacitor using carbon as an electrode material derived from PVC polymer. To fabricate a supercapacitor we have used electrolyte IL (1-ethyl-3-methylimidazolium thiocyanate) soaked in a filter paper and the specific capacitance we were getting above 120 F/g at 5 m V/s. We have also performed a stability test of a cell by measuring specific capacitance up to 15 days and up to 9000 cycles using cyclic voltammetry.

Keywords: Porous carbon, supercapacitor, cyclic voltammetry, low frequency impedance spectroscopy, ionic liquid.



Low frequency impedance spectra of prepared cell

SEM micrograph of prepared carbon

Structural, Microstructure and Dielectric Properties of La_2NiMnO_6 Double Perovskites Ceramics

Vijayeta Pal*, Chandra Bhal Singh, Dinesh Kumar and
Akhilesh Kumar Singh

School of Materials Science & Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi 221005, India
*E-mail: vijayetapal@gmail.com

Abstract

This study reports the preparation of double perovskites La_2NiMnO_6 ceramics by using high energy ball milling method. The structural, microstructure and dielectric properties of La_2NiMnO_6 ceramics were studied systematically. The phase formation and crystal structure of La_2NiMnO_6 ceramics were characterized using X-Ray diffraction technique. The micrograph shows the near-spherical grains in La_2NiMnO_6 ceramics. The temperature dependent dielectric study demonstrates relaxor-like dielectric behavior coupled with a giant dielectric constant. The unique dielectric characteristics should be ascribed due to the charge ordering of Ni^{2+} and Mn^{4+}.

Keywords: Double perovskite, Crystal structure, Microstructure, Dielectric Properties.

Influence of co-doping on Structural, Morphological, and Electrical properties of Ruddlesden-Popper-type $SmSrNiO_{4-\delta}$as a cathode material for IT-SOFC

Manisha Chauhan*,**Jay N. Mishra, Priyanka A. Jha, Pardeep K. Jha and Prabhakar Singh***

Department of Physics, Indian Institute of Technology (Banaras Hindu University) Varanasi (U.P), India
*****Email: manishachauhan.rs.phy17itbhu.ac.in; psingh.app@iitbhu.ac.in

Abstract

For electric power generation Solid Oxide Fuel Cells (SOFCs) is the promising technology. Ruddlesden Popper type rare earth Nickelates have shown better performance as cathode with various electrolytes such as SDC and YSZ. In the present work, Strontium Samarium Nickelate ($SmSrNiO_{4-\delta}$)and co-doped $Sm_{0.95}La_{0.05}Sr_{0.95}Ca_{0.05}NiO_{4-\delta}$were synthesized by solid state route at sintering temperature 1250 ˚C. The phase purity of samples is determined by X-Ray Powder diffraction method and further confirmed by Rietveld refinement which was performed using FULLPROF suite with *I4/mmm* symmetry and χ^2 lies appreciably within the experimental errors. The porous microstructure has been observed for all the studied samples. The conductivity is observed to increase nearly two folds with the co-substitution as compared to the parent sample. However, the oxygen reduction reaction is nearly same for both the samples.

Keywords: SOFC, Ruddlesden Popper Perovskites.

To study DC Conductivity and Dielectric properties of composition [PVA:CS:PEG]-$AgNO_3$ based biopolymer electrolyte films

Raghubir Kumar Prajapati, **A. L. Saroj and Horesh Kumar**

Department of Physics, Institute of Science, BHU Varanasi - 221005

Abstract

Biopolymer blend electrolytes (BPBEs) based on [PVA: CS: PEG]–xwt%$AgNO_3$ (x=0, 10, 20, 30, 40) viz. BPBE-1 to BPBE-5, respectively were prepared using solution cast method. Structural characterization has been performed using FTIR measurement. Electrochemical impedance spectroscopic (EIS) technique was used to study the ion transport mechanism of the studied samples. The electrochemical stability window (ESW) of the optimized sample was studied with help of linear sweep voltammetry (LSV) and cyclic voltammetry (CV) measurements. Ionic transference number (ITN) measurements were performed to study the nature of charge carriers present in the polymeric network. Temperature dependent dc conductivity (σ_{dc}) and dielectric relaxation frequency (f_r) for prepared samples follow the Arrhenius type thermally activated process. The dc conductivity value for optimized sample, BPBE-4 was found to be~ 1.7×10^{-4} S/cm at 30°C. The AC conductivity spectra of prepared samples follow the Jonscher's Power law (JPL) with the value of power law exponent, n<1.

Keywords: Ionic conductivity, Dielectric properties, ITN, CV

References:

[1] F.M. Gray, Solid Polymer Electrolytes–Fundamentals and Technological Applications, VCH, New York, 1991.

[2] Fernicola, A.; Scrosati, B.; Ohno, H. Potentialities of ionic liquids as new electrolyte media in advanced electrochemical devices , Ionics 2006, 12, 95.

[3] S.K. Chaurasia, R.K. Singh, and S. Chandra, J. Polym. Sci. Part B Polym. Dielectric relaxation and conductivity studies on (PEO:$LIClo_4$) polymer electrolyte with ionic liquid [BMIM][Pf_6] Phys. 49, 291 (2011)

[4] Galinski, M.; Lewandowski, A.; Stepniak, I. Electrochim. Ionic liquids as electrolytes Acta 2006, 51, 5567.

Synthesis and Photoluminescence Studies of Lanthanide Doped $Ca_9Y(VO_4)_7$ Polycrystalline Material

Manisha Sharma, Prof. Prabhakar Singh

Department of Physics, Indian Institute of Technology (Banaras Hindu University), Varanasi 221005, India

Abstract:

With the emergence of nanotechnology, lanthanide doped up conversion nanoparticles gradually become inevitable in varieties of application.$Ca_9Y(VO_4)_7$:Yb3^+/Er$3^+$is one of the ideal host having high chemical stability, thermalstability, low toxicity and high second harmonic generation efficiency. In the present work, it is synthesized by combustion method, XRD analysis of the material well matched with its jcpds file(#460411). The FTIR studies shows the strong peak at 820cm^{-1} which is associated with the vibrational mode of V-O bond. It's up conversion spectra shows bright green light emission upon a 980nm laser excitation.

Electrical Properties of $La_xSr_{1-x}TiO_{3-\delta}$ as SOFC Electrode Material

Uma Sharma and Prabhakar Singh*

Department of Physics, Indian Institute of Technology (BHU), Varanasi 221005

*Email: psingh.app@iitbhu.ac.in

Abstract

Lanthanum Strontium Titanate Oxide $La_xSr_{1-x}TiO_{3-\delta}$ (x = 0.5) with perovskite structure is one of the promising materials to work as an excellent anode in intermediate temperature solid oxide fuel cells (IT-SOFCs). In the present work, the composition with x = 0.5 was synthesized via solid state reaction route (SSR). The X-ray diffractograms revealed that it is crystallized in cubic ($Pm\bar{3}m$) structure and is in accordance with the reported results. Electrical properties are studied in the frequency range 1Hz to 1MHz and temperature RT to 700°C. The I-V characteristics showed the increase in leakage current at room temperature in $La_xSr_{1-x}TiO_{3-\delta}$.

Synthesis and Characterization of Modified Moringa Olifera Seed Pod Nanocellulose Based Hydrophobic Polyurethane Xerogels

Jyothy G Vijayan, T. Niranjana Prabhu and Jineesh A.G

Department of Chemistry, M.S. Ramaiah University of Applied Sciences, IV Phase, Peenya Industrial Area,
Bengaluru-560058, INDIA
Corresponding Author Email: jyothyvijayan.res.msruas@gmail.com

Abstract

In this study different weight percentage (1,3 &5) of modified Moringa Olifera seed pod nanocellulose based PU xerogels with different polyol components such as PEG 6000, seed oil based polyol (chaulmoogra and grape) were synthesized and characterized. The prepared nanocellulose and modified nanocellulose samples were characterized by using XRD, SEM, FTIR and FE-SEM. Hydrophobic PU-Xerogels were characterized by using SEM and ATR-IR. From XRD crystallinity index of the samples were found out. The SEM results show that the brittleness of the modified nano-cellulose filled polyurethane xerogel (mNC-PUXe) increased with the increase in the mNC-content. Thus, the crystallization of the PU molecular chains was promoted and it leads to the rigidity of the system. From ATR IR it was found that after mixing with modified nanocellulose, the mNC peaks no longer existed and were replaced by peaks belonging to the PU component. The results showed that varying nanocellulose content influences the synthesis and flexibility of the xerogels prepared.

Keywords: Polyurethane xerogels, modified nanocellulose (mNC), FESEM, XRD FTIR and hydrophobicity

Backup Phase Assisted $MnTiO_3$ Electrodes for Supercapacitor Applications

D. Lakshmi[1], M. Infanta Diana[1], R. Saranya[1], T. Kiruthika[1], P. Christopher Selvin[1*]

[1]Luminescence and Solid State Ionics Laboratory, Department of Physics, Bharathiar University, Coimbatore-46, Tamilnadu
* Corresponding Author Email: csphysics@buc.edu.in

Abstract

Perovskite based electrodes possess high range of electrical conductivity and structural stability as anodes for energy storage devices, especially for supercapacitors. In the present case, $MnTiO_3$ perovskite electrode was synthesized by solid state reaction method and analyzed for different properties. From XRD analysis, in addition to $MnTiO_3$ perovskite rhombohedral phase, tetragonal TiO_2 phase is also observed. Morphological analysis reveal the 1D spherical distribution of the samples. Elemental composition of the sample is estimated by Energy Dispersive X-ray analysis. Cyclic voltammetry and charge discharge analysis show ~815 Fg^{-1} specific capacitance of the $MnTiO_3$ sample when cycled for high numbers. The high value of capacitance observed is attributable to the secondary phase TiO_2 witnessed in the $MnTiO_3$ matrix which acts as a supplementary phase for performance enhancement of the host. Similarly, impedance analysis shows the electrical conductivity of the sample is in the order of 10^{-4} Scm^{-1}. Overall, the prepared $MnTiO_3$ sample is said to serve well in supercapacitor assembly.

Keywords: perovskite; electrode; supercapacitor; charge-discharge analysis; dual phase.

Design of Two Novel Dyes Having Maximum Absorption in Infrared Region: A DFT Investigation

Tabish Rasheed[1], Ankit Kargeti[1], Shamoon Ahmad Siddiqui[2,3]

[1] School of Engineering and Technology, BML Munjal University, Gurugram, Haryana, India 122413.
[2] Promising Centre for Sensors and Electronic Devices, Najran University, Najran, KSA 11001.
[3] Department of Physics, Najran University, Najran, KSA 11001.

Abstract

In recent times, dye sensitized solar cells (DSSCs) have been widely investigated by researchers and scientists. Grätzel et.al. [1]in 1991 designed the first DSSC based on Ruthenium complex. Since then, metal-free DSSCs have attracted the interest of researchers and have achieved efficiencies of 10-15%. In present work, two novel dyes have been designed based on D-π-A (Carbazole-Thiophene-Naphthalimide) and D-π-A-A (Carbazole-Thiophene-Naphthalimide-Benzothiadiazole) architectures (D, π and A represent donor, π bridge and acceptor respectively). Both the dyes have same donor and bridge elements, which are carbazole and thiophene respectively. The acceptor in first dye is naphthalimide and in second dye it is naphthalimide and benzothiadiazole. Geometries of the two dyes have been optimized under the framework of density functional theory (DFT) at B3LYP/ccPVDZ level using *Gaussian 16W*package. The results indicate that the absorption region of the two dyes lie in infrared region. The maximum absorption wavelengths of the dyes are 1432 nm (Carbazole-Thiophene-Naphthalimide) and 1351nm (Carbazole-Thiophene-Naphthalimide-Benzothiadiazole). Other relevant parameters such as light harvesting efficiency, charge injection energy, dye regeneration energy and open circuit voltage have also been calculated for the designed dyes.

Reference:

[1] B. O'Regan, M. Grätzel, Nature. 353 (1991).

Rechargeable Alkali Metal Ion Batteries with Chemically Reduced $Fe[Fe(CN)_6]$ Cathode

Dona Susan Baji, Shantikumar Nair, Dhamodaran Santhanagopalan*

Centre for Nanosciences and Molecular Medicine, Amrita Vishwa Vidyapeetham, Ponekkara, Kochi, India 682 041
Email: dsgopalan20710@aims.amrita.edu

Abstract

Prussian blue and its analogues (PBA) have been captivated due to its promising structural framework which can undergo interstitial alterations and substitution. This open frame work of PBA leads to good kinetics for even larger cations [1-3]. A simple, sustainable approach of chemical reduction of two prominent alkali metal ion containing $Fe[Fe(CN)_6]$ for lithium and sodium ion battery applications have been achieved. The single iron source prepared $Fe[Fe(CN)_6]$ has been undergone to a rapid chemical reduction that forms $Li_xFe[Fe(CN)_6]$ and $Na_xFe[Fe(CN)_6]$ at low temperature of 80°C under ambient atmospheric condition. The electron micrograph of these were recorded and confirmed the cuboid morphology which remained unaffected for the sodiation and lithiation process. As iron and sodium being abundant the major goal of this work is to fabricate alkali ion cathodes. Further in depth analysis of electrochemical rate performance, cycling stability of lithiated and sodiated $Fe[Fe(CN)_6]$ were evaluated. Poor lithiation led to low first charge capacity however, relatively better sodiation and 70% retention for 500 cycles at 100 mA/g was recorded. The electrochemical performance has been correlated by the *ex-situ* XRD for sodium ion battery with a cubic to monoclinic phase transition beyond 1st cycle was observed. Such a scalable, rapid and convenient chemical sodiation process of PBAs would make it an ideal cathode for Na-ion batteries.

Keyword: Chemical reduction, sodium ion battery, lithium-ion battery, Phase transition, *Ex-situ* analysis.

References:

[1] Q Li., Z Hu, et al., Advanced Functional Materials, 30(14), 1909530.(2020) https://doi.org/10.1002/adfm.201909530
[2] S.Yu,y.Li et al. Journal of Power Sources, 275,.45-49.(2015) https://doi.org/10.1016/j.jpowsour.2014.10.196
[3] Q J.Qian, C.Wu et al. Advanced Energy Materials, 8(17), 1702619(2018) https://doi.org/10.1002/aenm.201702619

Lithium-Rich Layered Cathode for Advanced Lithium-ion Batteries – Particle Size and Operation Temperature Effects

Silpasree S Jayasree, Shantikumar Nair and Dhamodaran Santhanagopalan*

Centre for Nanosciences and Molecular Medicine, Amrita Vishwa Vidyapeetham
Kochi 682 041, India.
*Corresponding author: dsgopalan20710@aims.amrita.edu

Abstract

Lithium-rich (LR) transition metal oxides have gained significant interest as advanced Li-ion battery cathode. Low initial coulombic efficiency, voltage fade, electrolyte decomposition and poor rate performance are the factors that hinders its commercialization [1, 2].Herein, we demonstrate the dependence of particle size and the operating temperature on the electrochemical performance of $Li[Li_{0.2}Ni_{0.2}Mn_{0.6}]O_2$ synthesized via sol-gel technique. LR cathode with a particle size of about 40 nm (named as LR_40), exhibited better cycling stability at 1 A/g over 250 cycles than the material with a particle size of ~ 150 nm (named as LR_150). Importantly, first cycle Coulombic efficiency at 125 mA/g was 78% which is a reasonably high value reported for LR materials, its cycling stability at both low and high rates have been noteworthy (~79% retention after 250 cycles at 1 A/g). Even at an elevated temperature of 55 ºC and a current density of 500 mA/g, LR_40 exhibited good cycling stability (~74% retention at the end of 100 cycles). The enhanced performance of LR_40 is attributed to the smaller particle size that enables the faster Li-ion diffusion kinetics. Surface-engineering to improve the electrochemical performances further by suppressing the oxygen release and voltage fade during cycling is proposed.

Keywords: Li-Rich cathode, Nanoparticles, Elevated stability, Li-ion battery.

References

1. Puheng, Yang, et al. "Self-standing $Li_{1.2}Mn_{0.6}Ni_{0.2}O_2$/graphene membrane as a binder-free cathode for Li-ion batteries." *RSC Advances* 8(2018): 39769-39776.
2. Liu, Haodong, et al. "Understanding the role of NH_4F and Al_2O_3 surface co-modification on lithium-excess layered oxide $Li_{1.2}Ni_{0.2}Mn_{0.6}O_2$." *ACS applied materials & interfaces* 7 (2015): 19189-19200.

Monthly Energy Yield Assessment of Solar photovoltaic System under Uniform Irradiance and Partial Shaded Conditions

Niti Agrawal[1,2], Avinashi Kapoor[2], Mridula Gupta[2]

[1]Department of Physics, Shyamlal College, University of Delhi, Delhi-110032, India
[2]Department of Electronic Science, University of Delhi South Campus, New Delhi- 110021, India

Abstract

Energy yield of an installed solar photovoltaic (PV) system depends on environmental and climatic condition of the location. Since an installed PV module experiences different conditions of temperature, irradiance, wind speed, solar spectrum etc., therefore how much energy a PV module will generate in the field is not fully understood by its name plate rating. This is because PV manufacturers rate the modules at only standard test conditions (STC) of 1000 W/m^2 and 25^{o}C. Estimating PV energy yield is of practical importance especially from the point of view of solar project developers and end customers. Moreover, partial shading condition which is an inevitable situation for the PV panels installed in the field, can seriously degrade the energy yield. The main objective of the present work is to assess the energy yield of the photovoltaic system under uniform irradiance and partial shading condition. The work highlights the adverse impact of partial shading on the energy yield. For this purpose, a PV system of polycrystalline silicon of rating132 Wp has been installed in the National Institute of Solar Energy, Gurugram, India. I-V data has been collected in real operating conditions to estimate the PV maximum output power at different conditions of irradiance and temperature under uniform irradiance as well as partial shading condition. Further, weather data for one complete year for the location is also obtained. Using the obtained set of data, monthly PV energy yield is estimated under uniform irradiance and partial shading condition. It is found that maximum energy is generated in the month of March and least in the month of July under uniform as well as partial shading condition. But under partial shading conditions, the energy yield is reduced to ~50%.

Keywords: solar photovoltaic, partial shading, energy yield, weather data

Band Gap Engineering of Batio$_3$ Perovskite Oxide by Vanadium Doping and Observation of Photovoltaic Response

Chandra Bhal Singh[1, a), Dinesh Kumar and Akhilesh Kumar Singh[1]

[1]School of Materials Science & Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi 221005, India
[a)]Corresponding author Email: cbs.sbc@gmail.com

Abstract

In recent years, the huge interest towards ferroelectric perovskites in photovoltaic area is observed due to its specific outcomes such as large-scale materials availability, potential for polarization driven charge carriers separation, high open circuit voltage and chemical stability. In this study, we demonstrate the synthesis of pure and vanadium (V) doped $BaTiO_3$ ferroelectric ceramics by conventional mechano-chemical ball milling process. X-Ray diffraction measurement confirmed the formation of phase-pure perovskites except highly V-doped $BaTiO_3$ ceramics. The vanadium doping affect the grain growth and results in increase in oxygen vacancies. The optical band E_g of the $BaTiO_3$ ceramics decreases by Vanadium doping and exhibit the lowest value (E_g= 1.65 eV) for 7% V_2O_5 doping. Further doping of V_2O_5 increase the band gap value and also reduce the ferroelectric polarization. The material show two different direct band gap features. The photovoltaic properties of V-doped $BaTiO_3$ (BTVO) ceramics were investigated. Very thin sintered pellets of BTVO were used to study photovoltaic effect and anomalous photovoltage is observed. The present study offers a new system of BTVO as photovoltaic materials.

Keywords: Perovskite oxide, Band-gap, Vanadium, Photovoltaic device, Energy Conversion

Carbon Captivated Nasno$_2$ Anode for Na-Ion Batteries

M. Infanta Diana[1], D. Lakshmi[1], P. Adlin Helen[1], P. Christopher Selvin[1*]

Luminescence and Solid State Ionics Laboratory, Department of Physics, Bharathiar University, Coimbatore – 641 046, Tamil Nadu
Corresponding author's E-mail: *csphysics@buc.edu.in

Abstract

A novel carbon-captivated NaSnO$_2$has been synthesized by carbonization of sodium alginate biopolymer by precipitation technique and appropriate calcination. The prepared sample NaSnO$_2$-C was analyzed by different physico-chemical and electrochemical properties for sodium-ion battery anode applications. XRD analysis reveals high crystallinity of the NaSnO$_2$ sample whereas a hump is observed at the lower angles as a result of carbon in the host matrix. The crystallite size of the sample is 18 nm as calculated by the Scherrer formula. Well refined morphology is observed for NaSnO$_2$-C sample by SEM analysis whereas elemental composition is elucidated by EDS analysis. The cyclic voltammetry and charge-discharge analysis reveal the good electrochemical activity of the prepared material. The structural stability issue of Na doped SnO$_2$ anode is subsidized in the present attempt by means of carbon encapsulation. Carbon acts as a controlled buffer matrix and protects the Na-SnO$_2$ anode from structural disintegration on repeated cycles. Further, owing to the large surface area by carbon and its high porous nature, the electrical conductivity has been improved and the value is in the order of 10^{-4} Scm^{-1} at room temperature. The high electrical conductivity value helps in the high rate capability of the anode for sodium-ion battery applications.

Keywords: sodium ion battery; alginate; electrode; charge-discharge; tin oxide.

Combustion Preparation of Reduced Graphene Oxide for Supercapacitor Application

A. Ramesh[1] and M. Sterlin Leo Hudson[2]*

[1,2]Hydrogen Energy Lab, Department of Physics, BHU, Varanasi-221005.
*Corresponding author: msterlinleo@gmail.com

Abstract

The facile one-step, cost-effective preparation of reduced graphene oxide by camphor-assisted combustion is reported for the first time. As a replacement for strong reducing agents and electrical furnace usage for reduction of GO, we reported a simple low-cost combustion method for GO reduction. The prominent feature of this work is that rGO derived thorough camphor assisted combustion process produce reasonable surface area with tunable porosity due to synthesis acquired carbon nanoparticles in rGO. The rGO derived from the combustion of GO exhibits a high specific capacitance of 241 Fg^{-1}. Which is higher than chemically reduced graphene oxide.

Reference:

A. Ramesh et al., *Dalton Transactions*, 2018, **47**, 5406–5414.

Effect of Ionic Liquid on Structural and Ion Transport Properties of CS-PVA-NaI Based Biopolymer Electrolyte Films

Devesh Chandra Bharati, A. L. Saroj

Department of Physics, Institute of Science, Banaras Hindu University, Varanasi- 221005
*****Email: deveshcbbhu93@gmail.com

Abstract

The loading effect of ionic liquid (IL), 1-ethyl-3-methylimidazolium methyl sulfate [EMIM][MS] on structural and ion transport properties of CS-PVA-NaI based biopolymer electrolyte films is investigated in this paper. The samples were made using the traditional solution cast method. The structural properties are determined by XRD, which reveals a significant variation in the characteristic peaks related to the semi-crystalline/amorphous phase of CS-PVA-NaI based biopolymer electrolyte films with different amount of IL loading. FTIR analysis reveals the interactions of polymer constituents with the dopant IL. To investigate the electrical transport properties of the prepared samples, the AC impedance spectroscopy technique is used. At room temperature, the sample containing 15% IL has the highest dc conductivity value of 1.72×10^{-4} S/cm. The electrode polarisation and conductivity relaxation were observed in IL base biopolymer electrolyte films based on dielectric permittivity and electric modulus studies. Ionic transference number (ITN) measurements have been used to investigate the nature of charge species, such as ionic or electronic. CV and LSV measurements were performed to determine the electrochemical stability window.

Keywords: Biopolymer, XRD, FTIR, Impedance spectroscopy, LSV & CV

Reference:

1. Pankaj Singh, D C Bharati, H Kumar and A L Saroj; Ion transport mechanism and dielectric relaxation behavior of PVA-Imidazolium ionic liquid based polymer electrolytes; Phys. Scr. 94 (2019) 105801 (9pp)
2. A L Saroj, R K Singh and S.Chandra Studies on polymer electrolyte poly(vinyl) pyrrolidone (PVP) complexed with ionic liquid: Effect of complexation on thermal stability, conductivity and relaxation behaviour;Materials Science and Engineering: BVolume 178, Issue 4 (2013) Pages 231-238
3. D C Bharati, Pooja Rawat and A L Saroj Structural, thermal and ion dynamics studies of PVA-CS-NaI based bio-polymer electrolyte films; Journal of Solid State Electrochemistry (2021) 25:1727–1741

Optimization of $MoSe_2$ Back Interface Layer for High Efficient CIGS Solar Cells: Numerical Analyses

Sachin V. Desarada, Nandu B Chaure*

Department of Physics, Savitribai Phule Pune University, Pune, 411007
***Email:** n.chaure@physics.unipune.ac.in

Abstract

$CuInGaSe_2$ (CIGS) is a promising candidate as an absorber material for thin-film solar cells. CIGS solar cell with 23.35 % efficiency was achieved by solar frontier group, which is maximum for any thin-film solar cell CIGS solar cell [1]. In conventional CIGS solar cell molybdenum was used as back contact. At high-temperature growth of CIGS, $MoSe_2$ layer gets formed at the Mo/CIGS interface [2]. While $MoSe_2$ layer is beneficial to form an ohmic contact between CIGS and Mo, in the excess amount, it could reduce the solar cell's performance due to the high resistance of $MoSe_2$. Properties of $MoSe_2$ were highly dependent on the deposition and processing method of CIGS, and can be modified to achieve maximum efficiency by improving Mo/CIGS junction properties. The effect of $MoSe_2$ layer was numerically investigated by using SCAPS-1D solar cell modeling software. By using a combination of energy bandgap from 1- 1.5 eV and thickness from 10 to 130 nm for $MoSe_2$ best configuration was determined for high-efficiency CIGS solar cell. By using $MoSe_2$ layer, efficiency was improved to 22.6 % with Voc of 0.74 V, Jsc of 3.6 mA/cm2 and fill factor of 0.89 from 14.55 % for cell without $MoSe_2$ layer. With in crease in the bandgap of $MoSe_2$, efficiency of the cell increased gradually up to 1.35 eV and then suddenly decreased for the bandgap above 1.35 eV. The decrease in efficiency is observed mainly because of the reduction in Jsc and reduction in FF due to lower maximum voltage output. As the thickness was increased from 10 nm up to 60 nm Jsc starts to increase due to reduction in recombination back contact and remains almost constant for thickness above 60 nm. Efficiency was observed to be improved with the thickness of $MoSe_2$ layer above 60 nm. With the increase of 8 % efficiency, the findings could be used to develop high efficiency, cost-effective CIGS solar cells.

Keywords: CIGS, $MoSe_2$, Simulation, SCAPS-1D

References:

1. (2019). Solar Frontier Achieves World Record Thin-Film Solar Cell Efficiency of 23.35%. Internet Solar Frontier.
2. Bermudez, V. and A. Perez-Rodriguez (2018). "Understanding the cell-to-module efficiency gap in Cu(In,Ga)(S,Se)2 photovoltaics scale-up." Nature Energy **3**(6): 466-475.

Enhancement in the Dielectric Properties in Rare Earth Cerium Doped Linbo$_3$ for High-Temperature Applications

Satyendra Kumar Satyarthi[1,2], Vishwa Pratap Singh[1,2], Akhilesh Kumar Singh[2]

[1]Department of Ceramic Engineering, Indian Institute of Technology (BHU), Varanasi, India[2] School of Material Science and Technology, Indian Institute of Technology (BHU), Varanasi, India
*Email: satyendraks.rs.cer17@itbhu.ac.in

Abstract

Environment friendly Lithium Niobate ($LiNbO_3$) is well known as very important Dielectric material. Which has rhombohedral symmetry and R3c space group at room temperature. The known Curie temperature (T_c) for LN at which ferroelectric-paraelectric transition occurs is about 1210°C. This material also possesses some other interesting characteristics like electro-optics and photo-refractive properties. In this work we have successfully synthesized Cerium doped Lithium niobate by high energy ball mill with milling speed 300 rpm. MgO sealed close chamber sintering process at 1100°C was performed to get dense pellets with good sintering characteristics. Structural analysis was done with the help of XRD and FTIR measurements. XRD analysis reveals that partial secondary phase forms due to Ce doping along with pure $LiNbO_3$ phase. Le-Bail profile matching analysis was done using Full prof suite software to analyze the crystal structure and determine structural parameters. Enhanced dielectric properties observed because of improved densification. Ferroelectric properties were investigated through Polarization-Electric field loop measurement. Enhanced dielectric properties of Ce-doped LiNbO3: (Ce) can be useful for capacitor-based device applications at high temperature.

References:

1. M. Manikandan et al. Journal of magnetism and magnetic materials 391 (2015) 156-160.
2. Abhai Mansingh et al. J. Phys. D: Appl. Phys. 18(1985) 2059-2071.

Influence of Filler Content on Magnesium Conducting Chitosan Biopolymer Electrolyte

P. Adlin Helen[a], P. Christopher Selvin[a]*

[a]Luminescence and Solid State Ionics Laboratory, Department of Physics, Bharathiar University, Coimbatore - 641046, India.
* Corresponding Author E-mail: csphysics@buc.edu.in (P.C. Selvin)

Abstract

The polymer electrolytes are one of the promising solid electrolytes in the pursuit of finding alternatives to commercially available liquid electrolytes and for the production of flexible and wearable battery applications. However the toxicity of synthetic polymers based on petroleum products are of great concern by researchers. Thus, biodegradable and ecofriendly biopolymer electrolytes are being studied to enhance its application for commercial use. Chitosan, a biopolymer obtained by deacetylation of chitin found in shrimp shells is the electrolyte under present study for its application in Magnesium batteries. To improve its overall properties different amounts of MnO_2 ceramic oxide filler in weight percentages have been added to the chitosan polymer host with 60 wt% of $MgNO_3.6H_2O$ salt. Especially improvement in the structural, thermal and conductivity properties on adding the filler have been widely studied and reported.

Keywords: Chitosan, Magnesium, filler, impedance, toxicity.

Catalytic Behaviour of Hydrothermal Processed NiO

Kamana Kumari Mishra*, Gargi, Prabhakar Singh*

Department of Physics, Indian Institute of Technology (Banaras Hindu University), Varanasi 221005, India
*Corresponding author: kamana.jra.phy21@itbhu.ac.in, psingh.app@itbhu.ac.in

Abstract

In the recent years most of the research is focused on the development of alternative source of energy viz., solar cell, fuel cells. Electrode is one of the major components for any kind of such cell or batteries. Electrodes generally require catalytic action and extensive literature survey reveals that there is utter requirement of efficient catalysts beyond the costly Pt catalyst. In the present work, Nanostructured Nickel oxide (NiO) were synthesized by Hydrothermal process by using Nickel Nitrate Hexahydrate $Ni(NO_3)_2.6H_2O$ and sodium hydroxide (NaOH) as starting material. The X-ray diffraction and Rietveld refinement analysis confirmed the phase of prepared nanoparticles. The band gap of the nanoparticles was estimated using UV-Vis spectra. The electrochemical measurements of the nanoparticles were done using cyclic voltammetry with different scan rates. Further, the chronoamperometric studies were used to demonstrate the reaction time as cathode material for fuel cell applications.

Keywords: Hydrothermal, NiO

One-Step Green Synthesis of $ZnFe_2O_4$ Anodes for Li Ion Batteries

T. Kiruthika[1], **D. Lakshmi**[1], **M. Infanta Diana**[1], **P. Adlin Helan**[1], **P. Christopher Selvin***[1]

[1]Luminescence and Solid State Ionics Lab, Bharathiar University, Coimbatore-46, Tamil Nadu
*Corresponding Author E-mail: csphysics@buc.edu.in

Abstract

The Zinc Ferrite ($ZnFe_2O_4$) spinel nanoparticles have been successfully prepared by green sol-gel synthesis mode employing Actinidia deliciosa fruit extract as reducing agent. The target application of the prepared material is anode part in Li ion batteries. The prepared $ZnFe_2O_4$ nanoparticles characterized by various analysis and the results are promising for this material to serve as anode in Li ion batteries. The structural analysis by means X-ray diffraction technique reveals phase pure cubic structure of this material with a crystallite size of 28 nm. The morphological pattern recorded by means of electron microscopes reveal cube shaped grains with mixed dimensions, within 50 nm. The Raman analysis clarifies the high crystalline nature of the prepared sample with sharp peaks. The absence of residues as a result of green reducing agents inside the $ZnFe_2O_4$matrix is ensured by means of absence of C-C peaks in FTIR spectra. The same has been verified by means EDX analysis which also reveals the presence of desired elements inside the sample matrix. The electrochemical activities and electrical conductivity values of the material seems to be positive towards the anodic application of $ZnFe_2O_4$ in Li ion batteries.

Keywords: Spinel; electrode; green synthesis; cyclic voltammetry; Li ion batteries.

Poly (Methyl Methacrylate) Doped with Ionic Liquid for Energy Storage Devices

Tejas Sharma[a,b], Pramod K. Singh[b]

[a]Department of Mechanical and Material Engineering, Universiti Tunku Abdul Rahman, Sungai Long Campus, Bandar Sg. Long, 43000 Kajang, Malaysia
[b]COE on Solar Cells and Renewable Energy, School of Basic Sciences and Research, Sharda University, Greater Noida 201310, India
Corresponding Author Email: sharma.tejas4@gmail.com (TS)

Abstract

In this work, a polymer electrolyte (PE) based on Poly (methyl methacrylate) PMMA doped with Ionic liquid (IL) 1-ethyl-3-methylimidazoliumtricyanomethanide (EMImTCM) was synthesized using solution cast method. The Addition of IL increases ionic conductivity and conductivity maximum (8.83×10^{-5} S cm^{-1}) observed at 30 wt.% of IL concentration in polymer. Polarized optical micrograph(POM), Fourier transform infrared spectroscopy (FTIR), and thermogravimetric analysis (TGA), X-ray diffraction (XRD) were also done to reveal the amorphous region, composite nature, thermal stability, crystalline nature respectively of developed IL-doped polymer electrolyte (PE) films. At last, we have used the maximum IL doped (30wt.%) in polymer matrix, film sandwiched in between carbon based electrodes (reported elsewhere by our group) to develop an efficient supercapacitor which confirms the specific capacitance 130 mF/g. The photovoltaic performance fabricated dye sensitized solar cell (DSSC) using same optimized polymer electrolyte was carried out at 1 sun condition which shows short-circuit current voltage of 0.61 V and an efficiency of 3.54%.

Preparation, Characterization and Application of Low Viscosity Ionic Liquid Doped Solid Polymer Electrolyte

Sushant Kumar[1,2], **Pramod K. Singh**[2], **Manoj K. Singh**[1]

[1]Department of Applied Science & Humanities, Rajkiya Engineering College Banda, Uttar Pradesh-210201, India
[2]Center of Excellence on Solar Cells and Renewable Energy, School of Basic Science and Research, Sharda University, Greater Noida, Uttar Pradesh-201306, India
Email: thekumarsushant@gmail.com

Abstract

Solid polymer electrolyte films blended with low viscosity ionic liquid in PVdF-HFP polymer are prepared via solution cast technique. The characterization of polymeric film is performed using X-ray diffraction (XRD), Polarized Optical Microscopy (POM), Fourier transform Infrared (FTIR) spectroscopy, and Thermo-gravimetric analysis (TGA) studies. The polymer electrolyte film with IL achieved conductivity as high as 10^{-2} S cm^{-1}. The electrical, structural and photoelectrochemical performance of polymer electrolyte are also presented in detail.

Keywords: Solid electrolyte, Conductivity, Relaxation Time, Dielectric loss, Electrochemical stability window

Electrical, Structural and Electrochemical Performance Of Polyethylene Oxide Doped With 1-Ethy-3-Methylimidazolium Tricynomethanide Ionic Liquid

Abhimanyu Singh[1], **Mustafa A. Alheety**[2]

[1]Department of Applied Physics, Gautam Buddha University, India
[2]Department of Nursing, Al-Hadi University College, Baghdad, Iraq
Corresponding Author Email: abhichess14@gmail.com

Abstract

In this paper, we have used polymer polyethylene oxide (PEO) as a host matrix and novel electrolyte ionic liquid 1-ethyl-3-methylimidazolium tricyanomethanide (TCM) as an dopant to increase ionic mobility. Different characterization techniques like Electrochemical impedance spectroscopy, dielectric measurement, Fourier transform (FT-IR), X-ray diffraction (XRD), polarized optical microscopy (POM), thermo-gravinometric analysis were used to identify the electrical, optical, structural and thermal properties. A laboratory scale supercapacitor has been fabricated using optimized SPE film as an electrolyte and porous carbon derived from corn starch which shows a specific capacitance 13.6 F/g at 50 mV/s scan rate.

Keywords: Solid polymer electrolyte, ionic liquid supercapacitor, cyclic voltammetry, specific capacitance.

Mg $(ClO4)_2$ Mixed Crosslinked Corn Starch: A Flexible and High Conducting Polymer-in-Salt-Electrolyte

Dipti Yadav[1] and Neelam Srivastava[1*]

[1]Department of Physics (MMV), Banaras Hindu University, Varanasi-221005, India
*Corresponding Author Email: neel@bhu.ac.in

Abstract

Polymer-in-salt-electrolytes (PISE) are a class of polymer-salt complexes which have greater amount of salt than host-polymer. In these electrolytes ion motion is decoupled from the segmental motion of host-polymer. Large concentration of salt results in a continuous ion-cluster throughout the matrix through which ion-transport occurs. Because of its predicted single and fast ion transport, many attempts have been made to synthesize it,but the literature indicates that unavailability ofsuitable polymer host to hold salt larger than its own amount and simultaneously keep it dissociated is still a great problem. PISE synthesis effortseither resulted in bad conductivity due to salt recrystallization or poor mechanical properties. Special stratagems are required to achieve anamorphous salt mixture,suitable for PISE synthesis. Only salts like LiTFSi or LiFSiresulted in PISEs with favorableproperties, but these saltsare quite costly. It is important to note that in PISEs amount of salt is quite large and hence its cost effectiveness isan important parameter.

In the present paper, a novel PISE system is being reported which neither requires complex method to identify a suitable salt complex nor any complex process/ instruments. It is synthesized using an environment friendly polymer (starch) crosslinked with Glutaraldehyde, $Mg(ClO4)_2$ is added to this using solution cast technique. The resulted electrolyte is not just highly conducting (5.67 x 10-2 S/cm) but is flexible and transparent. Moisture-content, FTIR, XRD and SEM analysis have confirmed that hydrogen bonding and high moisture content of the system play a vital role in achieving high conductivity along with flexible morphology. These systems give a new hope to see PISEs at commercial level.

Keywords: Polymer-in-salt-electrolytes, high-conducting, economical, environment-benign

Structural and Optical Investigations on Direct current (DC) magnetron sputtered CZTS thin film

Kalyan B. Chavan[1,2], Sachin V. Desarada[1], Nandu B. Chaure[1*]

[1]Department of Physics, Savitribai Phule Pune University (formerly University of Pune), Pune, 411 007, India

[2]Department of Physics, Ahmednagar College, Maharashtra, 414001, India

*Corresponding author Email: n.chaure@physics.unipune.ac.in

Abstract

Cu_2ZnSnS_4 (CZTS) claims a promising candidature in thin-film solar cells. Earth abundance and echo-friendliness of CZTS made it superior over CIGS absorber layers in TFSC [1]. In this article, we have reported the deposition of Cu_2ZnSnS_4 (CZTS) thin films on soda-lime glass (SLG) substrate by using DC magnetron sputtering. The deposition was preferred at different substrate temperatures from room temperature to 400°C at 50Watt DC sputtering power. 80 standard cubic centimeter per minute (SCCM) flow rate of Argon (Ar) was maintained during the 20 min. deposition. A quaternary Cu_2ZnSnS_4 (CZTS) target (Make: Testbourne Ltd, UK) having dimensions, 76.2 mm diameter x 6 mm thickness with 99.95 % purity was used. The sputtering chamber was evacuated to 10^{-6} mbar pressure. Thoroughly cleaned glass substrates were mounted on a substrate heater mount in a sputter chamber. The structural and optical measurements were performed using the x-ray diffractometer and UV-Vis-NIR spectrophotometer. CZTS thin film was deposited at room temperature shows amorphous nature. Enhancement in crystallinity of thin-film was noticed at higher deposition temperatures. Detailed structural probing was carried out with the help of Rietveld refinement using PROFEX refinement software. XRD patterns of CZTS thin films deposited at 200, 300, and 400°C portrays the change in the preferred orientation. A decrease in bandgap was observed upon increase in deposition temperature of CZTS thin films.

Keywords: DC Sputtering, CZTS thin films, XRD, Preferred Orientation, bandgap, etc.

References:

[1] M.Ravindiran, C.Praveenkumar, “Status review and the future prospects of CZTS based solar cell – A novel approach on the device structure and material modeling for CZTS based photovoltaic device”, *Renewable and Sustainable Energy Reviews,*Volume 94, October 2018, Pages 317-329.

Green synthesis of bismuth ferrite nanoparticle for PVA-PANI-BFO nanocomposite membrane to study the ionic conductivity with varying relative humidity

Diptarka Roy*[†], Kamlesh Pandey[‡], Anil Kumar Yadav[†]

[†]Department of Physics, Babasaheb Bhimrao Ambedkar University, Lucknow-226025, Uttar Pradesh, India.
[‡]National Centre of Experimental Mineralogy and Petrology, University of Allahabad, Allahabad-211002, Uttar Pradesh, India.
[*]Email: roy.arka.in@gmail.com

Abstract

Bismuth ferrite (BFO) nanoparticles were prepared using the green synthesis route, where Moringaoleifera leaf extract was used as a reducing and capping agent for the reduction of metallic ions during the nanoparticle synthesis process. The green synthesis route is beneficial due to its cost-effectiveness and eco-friendly nature. The green synthesized BFO nanoparticles were employed as nanofiller in PVA-PANI-BFO nanocomposite membranes. The synthesized BFO nanoparticles and PVA-PANI-BFO nanocomposite membrane were characterized by X-ray diffraction (XRD), Raman, and Fourier Transform Infrared (FTIR) spectroscopy. The surface morphologies of the synthesized nanoparticles and nanocomposite membrane were characterized by Field emission scanning electron microscopy (FESEM). Also, the elemental composition of the synthesized BFO nanoparticles was analysed by Energy Dispersive X-Ray Spectroscopy (EDS). The XRD pattern of the synthesized BFO nanoparticles confirms the phase of BiFeO3 with the rhombohedral crystal structure. The average crystallite size is calculated as 12.16 nm. The Raman spectrum indicates the characteristics bands of BFO. The FTIR spectrum indicates the existence of various organic compounds as the functional groups from the plant extract in the synthesized BFO. FESEM images show the size of the particles within the nanoscale, which is composed of mostly spherical and few disc-like structures. The effect of nanofiller in the PVA-PANI-BFO nanocomposite membrane was investigated relative to the PVA-PANI polymeric membrane. The membranes were synthesized by the solution cast method. The ionic conductivities of the membranes were investigated at different relative humidity. With changing the relative humidity (RH), the ionic conductivity of the membranes changed, indicated a clear influence of BFO nanofiller in the conductive polymeric membrane.