PEROVSKITE SOCIETY OF INDIA

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PROGRAMME AND ABSTRACTS

Perovskite Society of India Meet (PSIM) 2023

Indian Institute of Technology, Roorkee

Mar 1 - Mar 3

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A CONFERENCE ON

PEROVSKITE SOCIETY OF INDIA MEET (PSIM-2023)

Date: March 1-3, 2023
Venue: IIT Roorkee

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PEROVSKITE SOCIETY OF INDIA

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175 YEARS OF IIT ROORKEE
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Perovskite Society of India Meet (PSIM)-2023

March 1-3, 2023

Hosted by

Indian Institute of Technology, Roorkee, Roorkee
(Uttarakhand, India)

Organized by:

Indian Institute of Technology, Roorkee

&

Perovskite Society of India

Programme and Abstracts

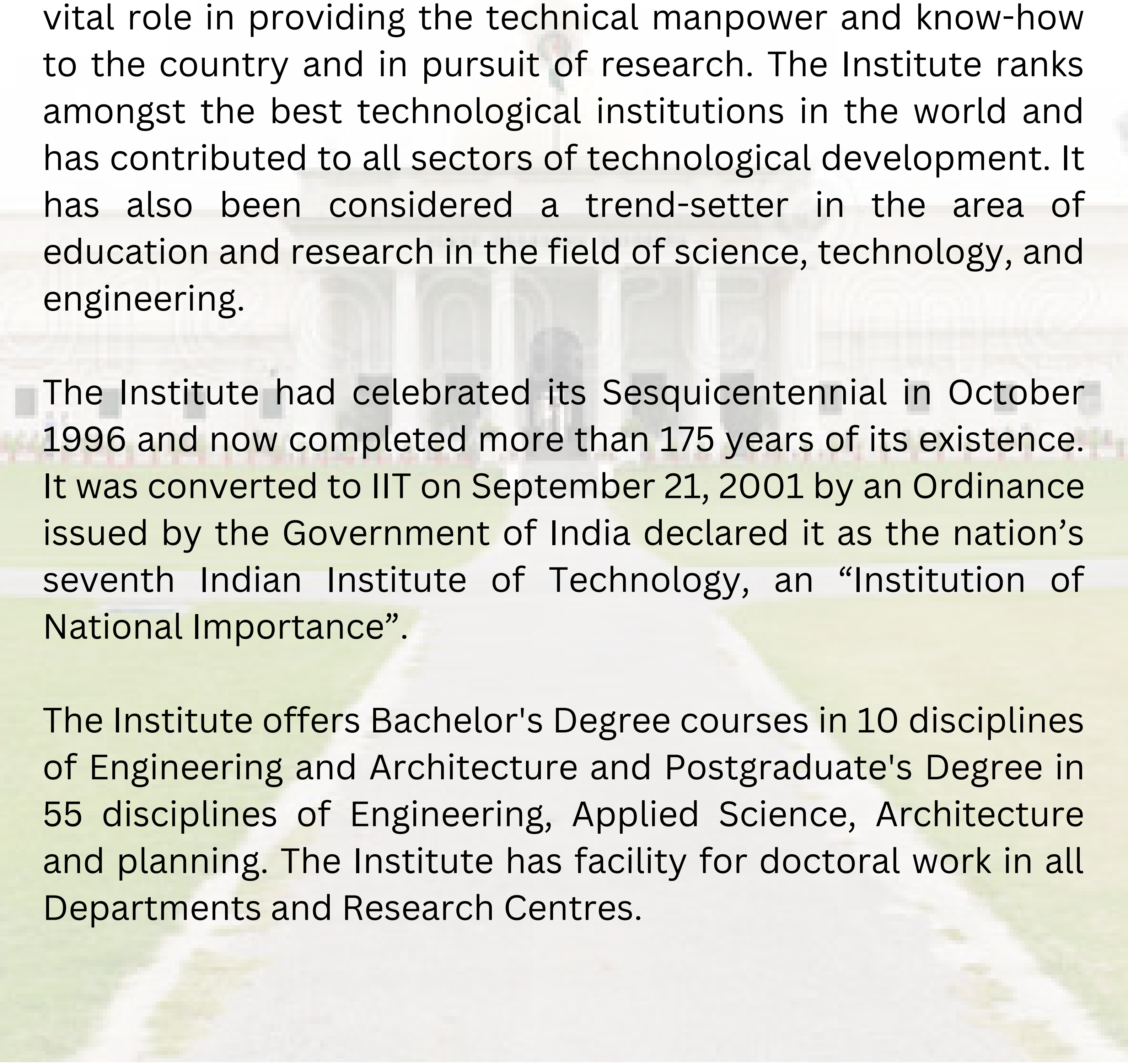
175 YEARS OF IIT ROORKEE Estd. 1847

PEROVSKITE SOCIETY OF INDIA

About PSIM-2023

In the past ten years, the hybrid metal halide perovskites has emerged as a new class of photovoltaics materials and sensor technology, they also provide fascinating opportunities for fundamental studies. The aim of this conference will be to provide a platform to interact and stimulate advancements in perovskite field both at lab and industry level. This conference will be designed to cover the three major research topics in the field of perovskite research including materials, devices and photophysics. The purpose of this meeting is to bring together experts on this topic, primarily within the country, working on various aspects of these materials. This conference will provide a platform to exchange knowledge about the latest academic and industry results and to discuss the latest trends, developments and limitations in perovskite photovoltaics.

About IIT Roorkee



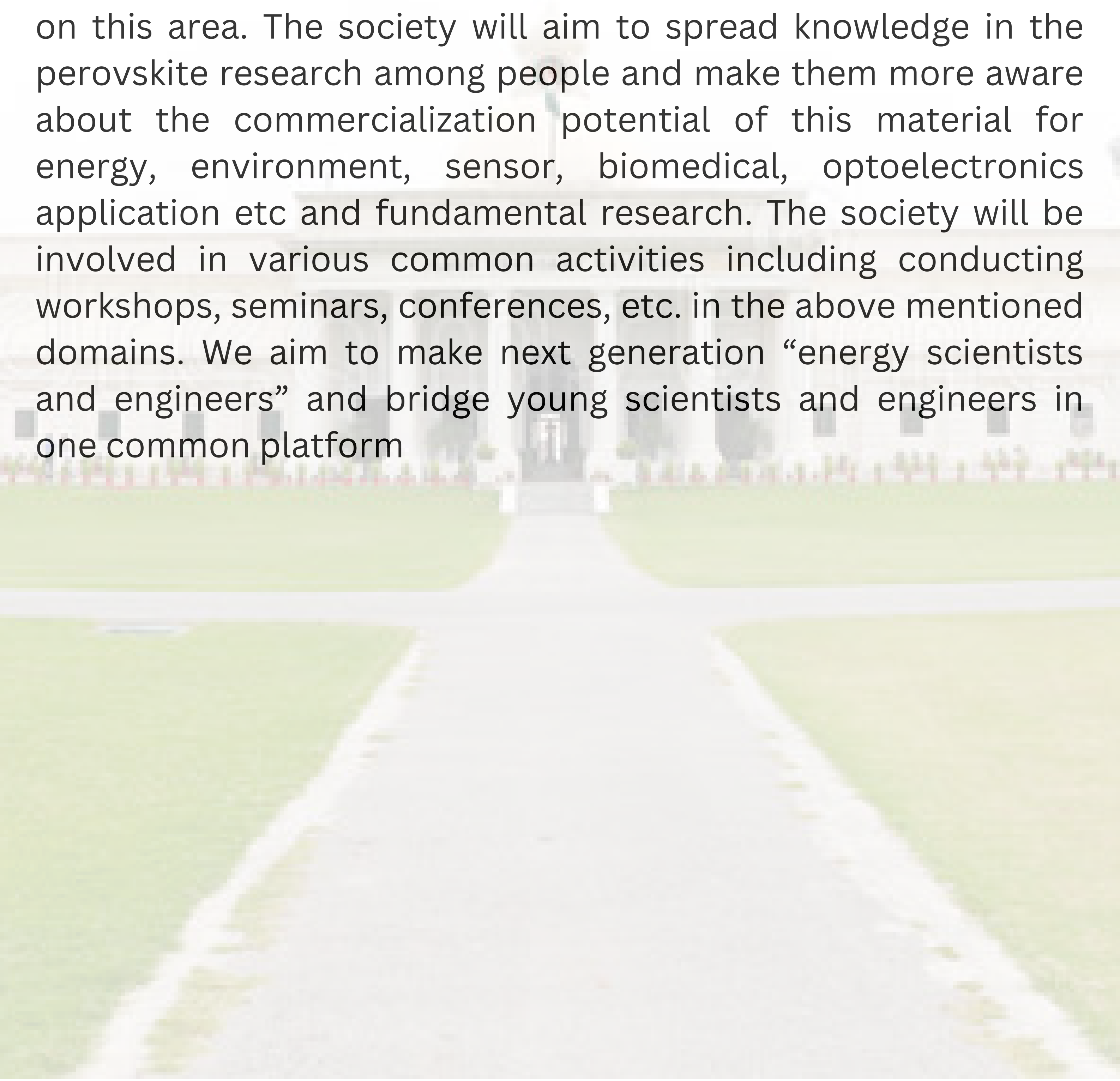
Indian Institute of Technology - Roorkee is among the foremost of institutes of national importance in higher technological education and in engineering, basic and applied research. Since its establishment, the Institute has played a vital role in providing the technical manpower and know-how to the country and in pursuit of research. The Institute ranks amongst the best technological institutions in the world and has contributed to all sectors of technological development. It has also been considered a trend-setter in the area of education and research in the field of science, technology, and engineering.

The Institute had celebrated its Sesquicentennial in October 1996 and now completed more than 175 years of its existence. It was converted to IIT on September 21, 2001 by an Ordinance issued by the Government of India declared it as the nation’s seventh Indian Institute of Technology, an “Institution of National Importance”.

The Institute offers Bachelor's Degree courses in 10 disciplines of Engineering and Architecture and Postgraduate's Degree in 55 disciplines of Engineering, Applied Science, Architecture and planning. The Institute has facility for doctoral work in all Departments and Research Centres.

About
Perovskite Society of India

One of the primary aim of the society will be to promote awareness about perovskite research and raise policy research on this area. The society will aim to spread knowledge in the perovskite research among people and make them more aware about the commercialization potential of this material for energy, environment, sensor, biomedical, optoelectronics application etc and fundamental research. The society will be involved in various common activities including conducting workshops, seminars, conferences, etc. in the above mentioned domains. We aim to make next generation “energy scientists and engineers” and bridge young scientists and engineers in one common platform

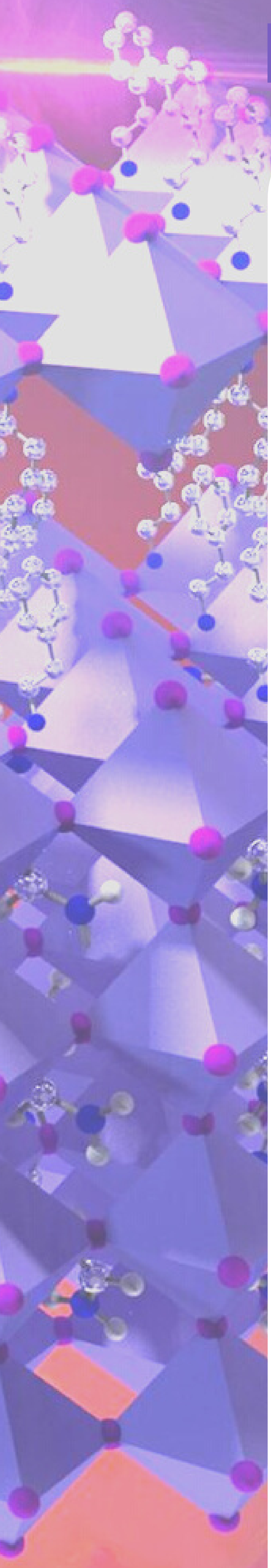


PSIM-2023 COMMITTEE

Patron	Prof. K. K. Pant
Advisory Committee	Prof. Narayan Pradhan Prof. Priya Mahadevan
Chairperson	Prof. G. D. Verma
Convener	Prof. Soumitra Satapathi

PROGRAM OVERVIEW

Day 1 : Wednesday, 1st March, 2023



08 : 00 AM onwards	Registeration
09 : 30 AM - 10 : 15 AM	INAUGURATION
10 : 15 AM - 10 : 45 AM	High Tea
10 : 45 AM - 11 : 30 AM	Panel Discussion
11 : 30 AM - 12 : 00 AM	Prof. Narayan Pradhan School of Material Sciences IACS, Kolkata Title - Charge transport in mixed metal halide perovskite semiconductors
12 : 00 PM - 12 : 30 PM	Prof. Sameer Sapra IITD Title - Coupling CsPbBr 3 perovskite nanocrystals with MoSe2 – a 2D transition metal dichalcogenide
12 : 30 PM - 01 : 00 PM	Prof. Priya Mahadevan S N Bose National Centre for Basic Sciences Kolkata Title - Can we have a set of rules to understand the structural distortions in 3-dimensional hybrid perovskites?
01 : 00 PM - 02 : 00 PM	LUNCH
02 : 00 PM - 02 : 30 PM	Prof. Dinesh Kabra IIT Bombay Title - Unconventional Materials that do more with Light
02 : 30 PM - 03 : 00 PM	Prof. Easwaramoorthi Ramasamy ARCI Title - Scalable Fabrication of Perovskite Solar Cells
03 : 00 PM - 03 : 30 PM	Prof. S.P. Singh CSIR Title – Rational Design of Π-Conjugated Small Molecules: From Structure to Function
03 : 30 PM - 04 : 00 PM	Prof. Ranjani Viswanatha JNCASR Title - Understanding mechanism of Mn emission in Perovskite halides using Raman Spectroscopy and Magnetic Circular Dichroism
04 : 00 PM - 05 : 45 PM	Poster Session & Tea break
05 : 45 PM - 06 : 15 PM	Dr. Giribabu Lingamallu CSIR Title - Alternative Holetransporting Materials for Perovskite Solar Cell
06 : 15 PM - 06 : 45 PM	Prof. Satyaprasad Senanayak NIISER Title - Charge transport in mixed metal halide perovskite semiconductors
06 : 45 PM - 07 : 30 PM	Plenary Speaker: Prof. Prashant V Kamat Department of Chemistry & Biochemistry University of Notre Dame, USA
07 : 30 PM - 08 : 15 PM	General Body Meeting
08 : 15 PM - 09 : 00 PM	Dinner

PROGRAM OVERVIEW

Day 2 : Thursday, 2nd March, 2023

08 : 15 AM - 09 : 00 AM	Breakfast
09 : 00 AM - 09 : 30 AM	Prof. Silvia Colella CNR Nanotec, Italy Title - Engineering hybrid halide perovskite processing and composition
09 : 30 AM - 10 : 15 AM	Prof. Hirendranath Ghosh BARC Title – Ultrafast Polaron Dynamics in Perovskite Materials
10 : 15 AM - 10 : 45 AM	Prof. Shaibal Sarkar IIT Bombay
10 : 45 AM - 11 : 00 AM	Prof. Sayan Bhattacharya IISER Kolkata Title – Dimensionality-control & Self-assembly of Perovskites
11 : 00 AM - 11 : 30 AM	Tea
11 : 30 AM - 12 : 00 AM	Prof. Sushobhan Avasthi IISC Bangalore Title – Dimensionality-control & Self-assembly of Perovskites
12 : 00 PM - 12 : 30 PM	Prof. Anshuman Nag IISER, Pune Title – Short-Wave Infrared (SWIR) Emitting (Doped) Halide Perovskites
12 : 30 PM - 01 : 00 PM	Prof. Prasun Mandal IISER Kolkata Title - Estimating Efficacy of Different Regions of the Solar Spectrum Towards Controlling Exciton Dynamics in Super-Bright, Highly-Pb-Replaced Perovskite Nanocrystal
01 : 00 PM - 02 : 00 PM	LUNCH
02 : 00 PM - 02 : 30 PM	Prof. Geetha Balakrishna Jain University, Bangalore Title - Suppression of Phase Segregation and Anion Exchange in Halide Perovskites towards Tandem Photovoltaics
02 : 30 PM - 03 : 00 PM	Prof. Arijit K De IISER Mohali Title - Mapping hot carrier relaxation mediated by low-frequency phonon modes in a lead-free double perovskite
03 : 00 PM - 03 : 30 PM	Prof. Janardan Kundu IISER Tirupati Title – Stereochemical Activity of ns2 Metal Ions & Dopants, Structure-Property Correlation, Host-Dopant & Dopant-Dopant Interaction in Low Dimensional Metal Halide Hybrids
03 : 30 PM - 04 : 00 PM	Prof. Zishan Husain Khan Jamia Millia Islamia, New Delhi.
04 : 00 PM - 05 : 45 PM	Poster Session & Tea break
05 : 45 PM - 06 : 15 PM	Prof. K.V.Adarsh IISER, Bhopal Title – Emergent Correlated Coherent Phenomena in Size and Shape Controlled Metal Halide Perovskite Quantum Dots
06 : 15 PM - 06 : 45 PM	Dr. Subhendu Kumar Panda CSIR-Central Title - Halide Perovskites: Promising Materials for Next Generation Renewable and Sustainable Energy Demands
06 : 45 PM - 07 : 30 PM	Prof. Pralay Santra(30mins) CeNS Bangalore
07 : 30PM - 08 : 15 PM	Gala Dinner

PROGRAM OVERVIEW

Day 3 : Friday, 3rd March, 2023

08 : 15 AM - 09 : 00 AM	Breakfast
09 : 00 AM - 09 : 30 AM	Prof. Deepa Khushalani TIFR Mumbai Title - Low Dimensional Hybrid Perovskites
09 : 30 AM - 10 : 15 AM	Prof. Vinod E. Madhavan NIT Calicut Title – Inorganic Hole Transport Material with 3D/2D Perovskite Solar Cells for higher stability
10 : 15 AM - 10 : 45 AM	Prof. Supravat Karak IIT Delhi Title - Understanding the different influences of host-salt non-stoichiometry, trap states and material phases on the performance of perovskite solar cells
10 : 45 AM - 11 : 00 AM	Dr. V Ganapathy Scientist, ARCI Title - Carbon based Perovskite Solar Cells for Scalability and Stability
11 : 00 AM - 11 : 30 AM	Tea
11 : 30 AM - 12 : 00 AM	Prof.D.D.Sarma Solid State and Structural Unit IISc Bangalore
12 : 00 PM - 12 : 30 PM	Prof. Ashish Kumar Sharma UPES Dehradun
12 : 30 PM - 01 : 00 PM	Prof. Rupak Banerjee IIT Gandhinagar Title - Mechanism of Ionic Conductivity, Dielectric Relaxation, and Energy Harvesting Properties of Halide Perovskites
01 : 00 PM - 02 : 00 PM	LUNCH
02 : 00 PM - 02 : 30 PM	Prof. Pankaj Yadav PDEU
02 : 30 PM - 03 : 00 PM	Prof. Shahab Ahmed IIT jodhpur Title - Metal Halide Perovskites: From Optoelectronic to Optoionic Devices
03 : 00 PM - 04 : 00 PM	Plenary Speaker: Prof. Osman Bakr (45 mins) Material Science and Engineering Kaust, Saudi Arabia
04 : 00 PM - 04 : 45 PM	Closing Ceremony
04 : 45 PM - 05 : 15 PM	Lab Visit

PLANERY TALKS

Plenary Talk

Prof. Prashant V Kamat

University of Notre Dame

Date: March 1

Time: 6.45 PM – 7.30 PM

Bio: Prof. Prashant Kamat is a distinguished Professor of Chemistry and Biochemistry and a Principal Scientist of Radiation Laboratory at University of Notre Dame. Prof. Kamat received his doctoral degree in Physical Chemistry from Bombay University, and carried out his postdoctoral research at Boston University and University of Texas at Austin. He is the editor-in-chief of the prestigious journal ACS Energy letter. He has received numerous awards including Thomson Reuters, Chemistry World, Indian National Science Academy and many more. The principle research interest of Prof. Kamat is nanotechnology and light energy conversion. Recently his research efforts have focused heavily on Quantum dot solar cell development.

Plenary Talk

Prof. Osman Bakr
KAUST

Date: March 3

Time: 2.30 PM – 3.00 PM

Bio: Prof. Osman M. Bakr is currently Professor of Materials Science and Engineering at KAUST, Saudi Arabia. He received his Ph.D. in Applied Physics from Harvard University. His research group focuses on the study of hybrid organic-inorganic nanoscale and bulk materials; particularly advancing their synthesis and self-assembly for applications in solar energy and optoelectronics. Presently he is an Associate Editor of ACS Materials Letters.

INVITED SPEAKERS

Invited Speaker

Prof. Narayan Pradhan

IACS

Date: March 1

Time: 11.30AM – 12.00PM

Bio: Prof. Narayan Pradhan is a distinguished Professor at India Association for the cultivation of Science. Prof. Pradhan received his doctoral degree from the Indian Institute of Technology (IIT), Kharagpur and carried out his post-doctoral research at Israel's Ben Gurion University and the University of Arkansas in the US. He has been a recipient of the LNJ Bhilwara Nanoscience award, the DST Swarnajayanti Fellowship award, the DST Nanoscience Young Career award, and the Oxford Nanoscientist. The principle research interest of Prof. Pradhan is Semicomductor and Doped Semiconductor Nanocrystals, Metal-semiconductor and Semiconductor-semiconductor Heterostructures, Photocatalysis using Hetero-Nanostructures, Multinary Semiconductor Nanostructures, PC and PEC water splitting.

Charge transport in mixed metal halide perovskite semiconductor

Abstract: Cesium lead halide perovskite nanocrystals are recently emerged as one of the most efficient energy materials for photovoltaics and light emitting devices. These nanocrystals with tuning their composition can tune the emission colors. Similarly, with proper reaction manipulations, these can lead to near unity photoluminescence quantum yields (PLQY) in all three prominent visible colors (Red, Blue and Green). These are mostly ionic character and hence, their synthesis and facet control indeed remained difficult in comparison to co-valent chalcogenide nanocrystals. Epitaxial growth of a second material or even secondary growth or shelling of different halide perovskite materials do not follow as simpler path as established with other nanocrystals. However, tuning their shape, facets and also dimensions are possible. Keeping importance of facet chemistry of halide perovskites, in this talk the formation pathways, phase stability, photoluminescence stability and facets tunability of different 3D halide perovskites and also their anisotropic structures will be presented. The use of Cs-sublattice structures for formation of different shape anisotropy and the correlation of exciton migrations in 1D shaped nanocrystals will also be discussed. Beyond normal nanorods or nanowires, spiraling in these halide nanostructures remained unique among all kinds of nanocrystals. Connections of cubes either via facets, edges or vortices can also be possible and in addition, their heterostructures with different inorganic as well as noble metal nanostructures also emerged with interesting chemistry and photophysical properties. From observing their formation in reaction flask to seeing those under electron microscope, all these features will be presented.

References:

S. Banerjee, S. Bera and N. Pradhan, ACS Nano 2023, 17, 678.
R. Das, A. Patra, S. K. Dutta, S. Shyamal, N. Pradhan, J. Am. Chem. Soc. 2022, 144, 18629.
S. Bera, S. Banerjee, R. Das and N. Pradhan, J. Am. Chem. Soc. 2022, 144, 7430.
S. Bera, S. Shyamal and N Pradhan, J. Am. Chem. Soc. 2021, 143, 14895.
S. Bera, R. Behera and N. Pradhan, J. Am. Chem. Soc. 2020, 142, 20865.
N. Pradhan, ACS Energy Lett. 2022, 7, 150.

Invited Speaker

Prof. Sameer Sapra

IIT Delhi

Date: March 1

Time: 12.00PM – 12.30PM

Bio: Prof. Sameer Sapra is Professor in Department of Chemistry IIT Delhi. Prof. mandal received his doctoral degree from IISc Bangalore and carried out his postdoctoral research at LMU Munich, and TU Dresden subsequently. He has received numerous awards and honours including, Outstanding Young Faculty Award (IIT Delhi), Alexander von Humboldt Fellowship. Prof. Sapra`s current research mainly focused on materials science, nanotechnology, quantum dots, charge separation and extraction, photocatalysis, photovoltaics.

Coupling $CsPbBr_3$ perovskite nanocrystals with $MoSe_2$ – a 2D transition metal dichalcogenide

Abstract: Exploring new optoelectronic properties necessitates preparation of heterostructures. Coupling $CsPbBr_3$ perovskite nanocrystals with the transition metal dichalcogenide (TMD) $MoSe_2$ nanosheets requires the use of a linker such as 4-aminothiophenol. In the presence of the linker a Type-II heterostructure forms, thus enabling charge separation between the perovskite and the TMD. Photodetectors with high ON-OFF ratios can be designed based on such heterostructures. The absence of a linker molecule does not result in a heterostructure; instead, the TMD completely disintegrates to form a passivation of PbSe over the $CsPbBr_3$ perovskite nanocrystals. These passivated structures enhance the stability of the perovskite nanocrystals tremendously.

References:

1. Enhanced Photocurrent owing to Shuttling of Charge Carriers across 4- Aminothiophenol Functionalized $MoSe_2$-$CsPbBr_3$ Nanohybrids Md. S. Hassan, P. Basera, S. Bera, M. Mittal, S. K. Ray, S. Bhattacharya, S. Sapra ACS Appl. Mater. Interfaces 12,7317 (2020).
2. Defect Passivation Results in Stability of Cesium Lead Halide Perovskite Nanocrystals Swati Khurana, Md Samim Hassan, Priyesh Yadav, Trupthi Chonamada, Manash R. Das, Pralay Santra, Dibyajyoti Ghosh, Sameer Sapra J. Phys. Chem. C 127, 3355 (2023).

Invited Speaker

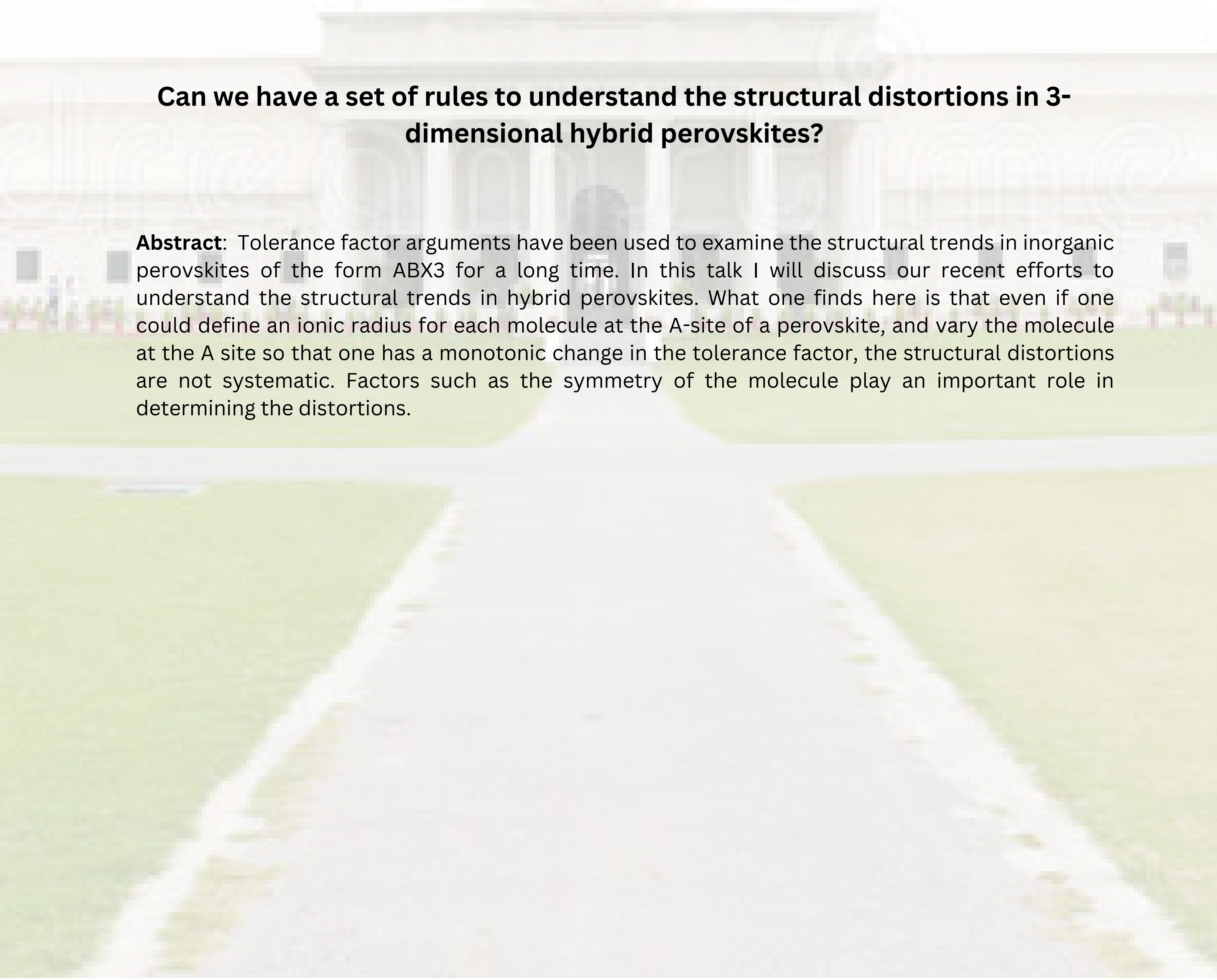
Prof. Priya Mahadevan

S.N. Bose National Centre for Basic Sciences, Kolkata

Date: March 1

Time: 12.30PM – 1.00PM

Bio: Prof. Priya Mahadevan is a Senior Professor of Condensed Matter Physics and Material Sciences in S.N. Bose National Centre for Basic Sciences at Kolkata. Prof. Mahadevan received her doctoral degree from IISc, Bangalore. Prof. holds a number of academic positions in India along with member of the editorial boards of several peer reviewed journals. Presently she is editorial Advisory Board member of ACS Energy Letters. She has received numerous awards including MRSI Medal, TWOWS Prize for young woman scientist. The principle research interest of Prof. Mahadevan is Electronic, magnetic, structural, optical and mechanical properties of systems at the nanoscale.



Can we have a set of rules to understand the structural distortions in 3-dimensional hybrid perovskites?

Abstract: Tolerance factor arguments have been used to examine the structural trends in inorganic perovskites of the form ABX3 for a long time. In this talk I will discuss our recent efforts to understand the structural trends in hybrid perovskites. What one finds here is that even if one could define an ionic radius for each molecule at the A-site of a perovskite, and vary the molecule at the A site so that one has a monotonic change in the tolerance factor, the structural distortions are not systematic. Factors such as the symmetry of the molecule play an important role in determining the distortions.

Invited Speaker

Prof. Dinesh Kabra

IIT Bombay

Date: March 1

Time: 2.00PM – 2.30PM

Bio: Prof. Dinesh Kabra is currently a Professor at the department of Physics, IIT Bombay. Prof. Kabra is faculty in-charge for emerging PV technologies at National Centre for Photovoltaic Research and Education (NCPRE) at IITB and also associated faculty member for Centre for Semiconductors for innovations and technologies (SEMIX). Prof. Kabra received his doctoral degree from Jawaharlal Nehru Center for Advanced Scientific Research, Bangalore. Thereafter, he pursued his post-doctoral research, from Cavendish laboratory at the University of Cambridge, UK. Prof. Kabra is recipient of DST Solar Challenge Award, Early Research Achiever Award and Best Paper Award of Industrial Research & Consultancy Centre, IIT Bombay. His research focus involves Energy Materials and devices, like; single junction & tandem Solar Cells, Transparent PV, In-door PV and optoelectronic devices. He is an expert in transferring the fundamental photo-physics and device physics of emerging photonic materials like halide perovskite and molecular semiconductors into the design of high-performance devices.

Unconventional Materials that do more with Light

Abstract: In this talk, I will give you an overview on the organic and halide perovskites semiconductors based activities taking place in our research group. [1] These semiconductors have emerged as potential photonics materials for future commercial optoelectronic devices, however, face a major challenge of ambient stability. Organic LEDs have become a matured technology by now for small display industries with budget crossing 10s B$. However, triplets are still a challenge, I will discuss one of in-depth study of triplet transport physics in organic semiconductors. [2] In halide perovskites; we have results of single junction cell PCE > 21% and silicon/perovskite tandem cell PCE > 26%. We also made LEDs with decent luminance efficiency ~ 25 cd/A. In halide perovskites, the two-dimensional (2D) and quasi-2D halide perovskites have shown promising stability against ambient stability. Hence, the understanding of the photo-physics of 2D perovskites can be a tool to get an in-depth insight into these novel halide perovskites. In this talk, I will discuss the origin of broadband illumination and other emission peaks using temperature- dependent time-resolved photoluminescence (PL) spectra of 2D layered halide perovskites (i.e., $(PEA)_2PbBr_4$ and $(PEA)_2PbI_4$) semiconductors. [3] Broad emission in $(PEA)_2PbBr_4$ perovskite is observed due to coupling of electronic states in inorganic well part ($PbBr_6^{4-}$) and organic barrier part (PEA), which is in contrast to a proposed model based on self-trapped-exciton.

References:

1. JM Crow "Unconventional materials that do more with light" Nature 608 (7924), 838- 838 (2022)
2. G.S. Banappanvar et al "Novel optoelectronic technique for direct tracking of ultrafast triplet excitons in polymeric semiconductor" Applied Physics Reviews Vol. 8, p-031415 (2021)
3. Laxmi and D. Kabra "Origin of Contrasting Emission Spectrum of Bromide vs Iodide Layered Perovskite Semiconductors" J. Phys. Chem. Lett. Vol. 13, p-2737 (2022)

Invited Speaker

Dr. Easwaramoorthi Ramasamy

ARCI

Date: March 1

Time: 2.30PM – 3.00PM

Bio: Dr. Easwaramoorthi Ramasamy is Scientist at Center for Solar Energy Materials, International Advanced Research Centre for Powder Metallurgy and New Materials (ARCI), Hyderabad. He received his doctoral degree from Korea University of Science & Technology and caried out postdoctoral research at Pohang University of Science and Technology (POSTECH), Korea . His Current research interests focused on Energy Conversion and Storage Technologies, Device Physics, Optoelectrical Characterization, Green Synthesis of Nanomaterials.

Scalable Fabrication of Perovskite Solar Cells

Abstract: Halide perovskite absorber based next generation solar cells (PSCs) reached a certified power conversion efficiency of 25.6%, a value comparable to that of silicon photovoltaics. Defect tolerance, high optical absorption and long carrier diffusion length are some of the intriguing properties made halide perovskite potential material for low-cost, high-efficiency next generation photovoltaics. Although lab-scale PSCs with high efficincies (> 20%) routinely fabricated by spin depostion, non-uniform precursor deposition and crystalization over large area substrate limiting the PSC module efficiency around 10%. This talk will provide comprehensive insight and our approach on materials and processes development for the fabrication of perovskite solar module. The importance of interfaces and associated losses will also be discussed. Strategies to improve PSC module's efficiency and operational stability through rational design of device architecture and encapsulation will also be presented.

Invited Speaker

Prof. Surya Prakash Singh

CSIR-Indian Institute of Chemical Technology, Hyderabad

Date: March 1

Time: 3.00PM – 3.30PM

Bio: Prof. S.P. Singh is a Principal Scientist at Polymers and Functional Materials Department, CSIR-Indian Institute of Chemical Technology, Hyderabad. Prof. Singh received his doctoral degree in chemistry at the University of Allahabad, India, and carried out his postdoctoral research at Nagoya Institute of Technology, Japan. Later, he joined CSIR-Indian Institute of Chemical Technology, Hyderabad as Research associate. He received AVRA Young Scientist Award in 2015. The principle research interest of Prof. Singh is Dye-Sensitized Solar Cells, Organic Solar Cells, etc.

Rational Design of Π-Conjugated Small Molecules: From Structure to Function

Abstract: Energy plays an essential role in social, economic and industrial improvement. Day-by-day in our daily life energy consumption is increasing. The energy demand is more due to this we are vastly using fossil fuel (petroleum, coal and natural gas) for energy production from past decades. These fossils fuel-producing carbon dioxide (CO2), which are subjective to global warming and environmental effects. Small organic molecules with suitable photophysical and electronic properties have attracted great attention towards Hi-tech applications based on photonic devices, such as dye sensitized solar cells, organic solar cells, emissive displays such as organic light emitting devices; electronic materials, such as organic semiconductors and security printing. Organic solar cells or organic photovolatics are emerging as one of the promising technologies for renewable energy sources because of their potential low-cost fabrication, color-tunable feature, and mechanical flexibility. Many research activities have endeavoured to develop new organic materials and device configurations for improving the efficiency and practical durability of the devices. Our research groups are actively demonstrating development of new and stable organic molecules for various applications. In this event, I will be presenting our recent development on hole-transport materials for perovskite solar cells. The talk will start with a brief introduction of solar cells followed by industrial application and commercialization of dye molecules.

Invited Speaker

Prof. Ranjani Viswanatha

JNCASR

Date: March 1

Time: 3.30PM – 4.00PM

Bio: Prof. Ranjani Viswantha is a distinguished Professor at JNCASR in Bengaluru. Prof. Ranjani received her doctoral degree from the Indian Institute of Science, Bangalore and carried out postdoctoral research at University of Arkansas and later at Los Alamos National Laboratory. The principal research interest of Prof. Ranjani's group focuses on synthesis of semiconductor nanocrystals and metal-semiconductor hybrid structures, along with studying optical and electronic properties of these materials.

Understanding mechanism of Mn emission in Perovskite halides using Raman Spectroscopy and Magnetic Circular Dichroism

Abstract: In this talk, we present a comprehensive study on the origin of Mn emission in Mn-doped perovskite halides using Raman spectroscopy and magnetic circular dichroism (MCD). By analyzing the Raman spectra, we demonstrate the influence of the local structural distortions and phonon modes on the Mn emission. In addition, we investigate the role of magnetic properties on the Mn emission by measuring the MCD spectra. Our results suggest that the Mn emission is strongly influenced by both the local structural distortions and magnetic properties of the host material. MCD shows the interaction of deeper levels of the conduction band and is severely affected by the spin orbit coupling. This study provides a deeper understanding of the Mn emission in perovskite halides and highlights the importance of considering both structural and magnetic properties in designing Mn-doped perovskite halides for optoelectronic applications.

Invited Speaker

Prof. Giribabu Lingamallu

CSIR-Indian Institute of Chemical Technology, Hyderabad

Date: March 1

Time: 5.40PM – 6.15PM

Bio: Dr. Lingamallu Giribabu is a distinguished Senior Principal Scientist at CSIR-Indian Institute of Chemical Technology, Hyderabad. Dr. Lingamallu Giribabu received his doctoral degree from University of Hyderabad, Hyderabad, and carried out his postdoctoral research at University of Houston, USA and later to Central Queensland University, Australia. He has received Associate Editor of Solar Energy (Elsivier). His principle research interest in the area of porphyrins and related molecules such as phthalocyanine, corroles etc., for synthesis, characterization, optical, electronic properties and their applications to solar energy harvesting and organic electronics.

Alternative Holetransporting Materials for Perovskite Solar Cell

Abstract: Perovskite solar cells have crossed device efficiency of 28%. However, the technology is not yet commercialized due constrains in materials. Among various components of the device, hole transporting maerials (HTMs) are play crucial role in achieving high efficiency and durability of the device. The widely used HTM is a metal-free organic compound, Spiro-OMeTAD. 1-3 In spite of showed such huge efficiency, Spiro-OMeTAD is very expensive due to tedious synthetic protocols as well as less durable towards thermal stress. Therefore, one has to look into the alternative HTMs. Our group particularly interested pigment based molecules such as sub- phthalocyanine, phthalocyanine, porphyrins and other tetrapyrrolic systems. We designed and synthesized several porphyrin based HTMs using donor-π-donor concept and because of hydrophobic nature these molecules the device is stable towards the moisture, which is one of the technical constrain of perovskite technology. The detailed design concept, synthesis, characterization and device studies will be presented.

Invited Speaker

Dr. Satyaprasad P Senanayak

NISER

Date: March 1

Time: 6.15PM – 6.45PM

Bio: Prof. Satyaprasad Senanayak is a distinguished Professor at National Institute of Science Education and Research. Prof. Satyaprasad received his doctoral degree from Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore. He has received numerous awards including Physical Science Research Council Global Challenge Research Award and many more. The principle research interest of Prof. Satyaprasad is Device Physics, Semiconductors, Charge Transport, Field Effect Transistors, Photovoltaics, Light emitting Diodes, Medical Diagnostic Devices.

Charge transport in mixed metal halide perovskite semiconductors

Abstract: Investigation of the inherent field-driven charge transport behaviour of three-dimensional lead halide perovskites has largely remained challenging, due to the undesirable ionic migration effects near room temperature and dipolar disorder instabilities. I will discuss how to address both these challenges and demonstrate that field-effect transistors using methylammonium-free, mixed metal (Pb/Sn) perovskite compositions which do not suffer from ion migration effects as notably as their pure-Pb counterparts and reliably exhibit hysteresis-free p-type transport with a mobility reaching 5.4 cm^2/Vs. The reduced ion migration is visualized through photoluminescence microscopy under bias and is manifested as an activated temperature dependence of the field-effect mobility with a low activation energy (~48 meV) consistent with the presence of the shallow defects present in these materials.

Invited Speaker

Prof. Silvia Colella

University of Bari

Date: **March 2**

Time: 9.00AM – 9.30PM

Bio: Prof. Silvia Colella is an academic researcher from University of Bari. Silvia Colella graduated in industrial chemistry in 2006 and took a PhD in Nanoscience in 2010. Since then, she has worked both in accademia and in industry, at the University of Muenster (Germany), Institute of supramolecular chemistry in Strasbourg (France), University of Salento (Italy) and BASF - The chemical company (Germany), building a strong expertise in the development of organic and hybrid semiconductors for optoelectronic applications, in particular photovoltaics. Since 2012 she is a senior scientist at the Institute of nanotechnology of the italian CNR, leading a group working in the field of perovskite-based photovoltaics. She has published more than 100 scientific works and 3 patents, collecting nearly 4000 citations.

Engineering hybrid halide perovskite processing and composition

Abstract: Metal halide perovskite (MHP) semiconductors are excellent candidates for contemporary optoelectronics innovation, particularly for photovoltaics. 1 The advantages of this class of materials derive from their hybrid nature, allowing for straightforward fabrication processes, and from their unique optoelectronic properties. A typical 3D organic-inorganic perovskite has a chemical formula of ABX_3, where A is an organic cation (such as MA [methylammonium] or FA [formamidinium]), B is a metal cation (such as Pb^{2+}), and X is a halogen anion (such as I or Br). 2 However, recent advances have also explored more complex compositions embedding diverse cations/anions. 3 In such a complex solution, it is important to study the stability of the ink and the existence of chemical reactivity between the components, in order to make inks ready for large scale applications. We provide insights into the complex solution chemistry of perovskite inks 4 and outline the directions towards which future research efforts should be directed. 5 . On the other hand, another way to act on the material stability and simplify the processing is adding a third component, an additive, to the mixture. We report on the advantages of polymeric additives for flexible photovoltaics and building integration. 6,7

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Invited Speaker

Prof. Hirendra N. Ghosh

BARC

Date: March 2

Time: 9.30AM – 10.15AM

Bio: Prof. Hirendranath Ghosh is a scientist at BARC. Currently Prof. Ghosh is an officiating director at INST Mohali. Prof. Ghosh received his doctoral degree from University of Bombay at Mumbai. Prof. Ghosh has won several prizes and awards for his work, including Homi Bhabha Science & Technology Award from Department of Atomic Energy in India, C. N. R. Rao National Prize for Chemical Research from Chemical Research Society of India, J.C Bose fellowship. His Research Interest focus on Ultrafast Photochemistry and Reaction Dynamics in solution phase and on nanostructured materials. Ultrafast charge carrier and interfacial electron and hole transfer dynamics in nanostructured and quantum dot core-shell materials using femtosecond visible, infrared and terahertz spectroscopy. And also Design and Development of Dye-sensitized Solar Cell and Quantum Dot Solar Cell using Fast and Ultrafast spectroscopic Techniques.

Ultrafast Polaron Dynamics in Perovskite Materials

Abstract: Polaron formation is widely acknowledged as the primary cause behind the retarded carrier relaxation observed in Metal Halide perovskites (MHPs), especially at low carrier densities. The key goal of this talk would thus be delivering an overview of the polaron dynamics in some optically relevant MHPs namely, $CsPbBr_3$, its modified versions, and emerging lead free systems in the framework of transient absorption and time resolved terahertz investigations. The generation and decay of polarons are influenced by a variety of experimental factors and intrinsic lattice properties, and these themes will be thoroughly reviewed. Excitation energy, lattice polarity, surrounding dielectric medium, lattice temperature, and system dimensionality etc. which influence the carrier- Longitudinal Optical phonon coupling responsive for driving the polaron formation will be addressed. I will also be discussing some of the most recent research from our group, including one in which we discovered that B-site doping had no impact on the polaron formation process in spite of expectations and another in which we observed the presence of polaron in a tin-based lattice. In conclusion, this talk will certainly provide a clear picture of the factors affecting polaron formation and how these can be used to steer the carrier relaxation rate for achieving improved functionality of the devices employing these materials.

Invited Speaker

Prof. Shaibal Sarkar

IIT Bombay

Date: March 2

Time: 10.15AM – 10.45AM

Bio: Prof. Shaibal Sarkar is a distinguished Professor at Department of Energy Science and Engineering, IIT Bombay. Prof. Sarkar received his doctoral degree from Weizmann Institute of Science, Israel, and carried out his postdoctoral research at Materials Research Center, University of Missouri at Rolla and later at University of Colorado at Boulder. Prof. Sarkar has been recipient of several fellowships and awards for his outstanding career in academic and research fields. The principle research of Prof. Sarkar group is focused broadly on Sensitized Solar cells, Photoelectrochemistry, Nanocrystalline Materials for Photovoltaic applications, Transparent Conducting Oxides, Atomic Layer Deposition.

Invited Speaker

Prof. Sayan Bhattacharyya

IISER, Kolkata

Date: March 2

Time: 10.45AM – 11.00PM

Bio: Prof. Sayan Bhattacharya is a distinguished professor of Materials Chemistry and Nanotechnology at Indian Institute of Science Education and Research (IISER) Kolkata. Prof. Bhattacharya received his doctoral degree in Solid State Chemistry from Indian Institute of Technology (IIT) Kanpur, and carried out his postdoctoral research at Drexel Nanotechnology Institute, Drexel University, Philadelphia, PA, USA. He has received SERB-STAR Award, Government of India, and Best paper award at National Symposium on Nanostructured Materials, IIT Delhi. The principle research interest of Prof. Bhattacharya is Electrocatalysis, Metal-Halide Perovskite Optoelectronics.

Dimensionality-control & Self-assembly of Perovskites

Abstract: Metal-halide perovskites with a soft ionic lattice have emerged as revolutionary optoelectronic materials in the recent years. While lead-based systems have made tremendous progress in photovoltaics, the lead-free counterparts are promising game-changers in optoelectronic devices and photocatalytic reactions. Some of our activities revolve around achieving "stable" perovskite solar cells with 20% photoconversion efficiency, employing the perovskite nanostructured films in photodetectors and field-effect transistors, alongside understanding the intriguing optical properties as a function of shape, size and composition of the lattice. In fact, the assembly, morphology, and structural changes of the perovskite nanostructures on solid substrates has a tremendous impact on the photoactive films. This lecture will discuss the metal-substitution induced 3D to 2D structural transformation of a lead halide perovskite, as well as the incessant light/dark reversible assembly of non-lead perovskite nanoplatelets.

Invited Speaker

Prof. Sushobhan Avasthi

IISC

Date: **March 2**

Time: **11.30AM – 12.00PM**

Bio: Prof. Sushobhan Avasthi is an assistant professor in the Indian Institute of Science at the Centre for Nano Science and Engineering (CeNSE), Indian Institute of Science (IISc). Prof. Avasthi received his doctoral degree from Princeton University, NJ, USA. He then worked as a post-doctoral research associate in the Princeton Institute of Science and Technology of Materials (PRISM). Sushobhan's current research interests are thin-film photovoltaics, heterojunction solar cells, and metal-oxide electronics. He has been awarded the prestigious Young Engineer Award for 2018 by the Indian National Academy of Engineers (INAE).

Dimensionality-control & Self-assembly of Perovskites

Abstract: It is now well understood that lead-halide perovskite solar cells are limited by surface recombination. In this talk I shall present our latest results in characterizing the interface of perovskite devices. We have built a novel photoelectromagnetic setup that is sensitive to carrier diffusion parameters of perovskite films. Using the technique, we have been able to directly measure diffusion length and surface recombination velocity in perovskite. We also use photoelectron spectroscopy to understand the band-alignment at perovskite/HTL interface. I shall present data on some new TPE based hole-transport devices.

Invited Speaker

Prof. Angshuman Nag
IISER, Pune

Date: March 2
Time: 12.00PM – 12.30PM

Bio: Prof. Angshuman Nag is currently a Professor at the department of chemistry, Indian Institute of Science Education and research, Pune. Prof. Anshuman received his doctoral degree from IISC Bangalore. Thereafter, he pursued his post-doctoral research, at the University of Chicago, USA. He has a long list of awards and accolades to his credit including Ramanujan Fellowship by DAT, DAE-BRNS Young Scientist Research Award, Young Associate of Indian Academy of Sciences, MRSI Medal. Currently he is the editorial Advisory Board Member of Chemistry of materials and Nano letters. Prof. Nag's research interest is on developing functional inorganic materials his group is focused broadly on Lead Halide perovskite, Lead free perovskite, Magnetically doped TCO and Surface modification.

Short-Wave Infrared (SWIR) Emitting (Doped) Halide Perovskites

Abstract: Short-Wave Infrared (SWIR) Emitting (Doped) Halide Perovskites Abstract - Short-Wave Infrared (SWIR, 900 to 1700 nm) radiations fall in the range between the typical electronic spectroscopy and vibrational spectroscopy. This wavelength region is transparent to most materials and molecules, resulting into applications in optical fibre, bio-imaging, and security camera. However, some of the vibrational overtones of –OH, –NH etc fall in this spectral region, and therefore can be utilized to verify food freshness/purity and related applications. At present, both SWIR detectors and SWIR light emitting diodes (LEDs) are fabricated by using epitaxially grown III-V semiconductors, with limitations in mass production and high expense. In this talk, I will discuss about potential of stable and Pb-free metal halide perovskites for applications in SWIR LEDs. For example, we dope lanthanides like Yb and Er in Cs 2 AgInCl 6 double perovskites that emit sharp SWIR radiation around 990 nm and 1540 nm (optical fibre communication region), respectively. 1,2 Then in order to achieve broad SWIR emission, that strongly overlaps with the vibration overtones of water, we have doped Cr 3+ into similar double perovskites. Furthermore, codoping of ions like Bi 3+ (that has two electrons in the outermost s-orbiatl) yields white light emission. 3 Also, OD perovskites like Cs 2 MoCl 6 exhibit broad SWIR emission with a small Stokes shift (and hence potentially high wall-plug efficiency). Phosphor converted LEDs (pc-LEDs) are fabricated for all these newly developed halide perovskite phosphors, demonstrating their usefulness in food freshness inspection.

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Invited Speaker

Prof. Prasun K. Mandal

IISER, Kolkata

Date: **March 2**

Time: 12.30PM – 1.00PM

Bio: Prof. Prasun Mandal is Professor & Principal Investigator in Department of Chemical Sciences IISER Kolkata. Prof. mandal received his doctoral degree from university of Hyderabad in fluorescence spectroscopy and carried out his postdoctoral research at Institut für Physikalische Chemie, Johannes Gutenberg Universität, Mainz, Germany and Vincent Croquette - ENS – PSL Paris, France subsequently. He has received numerous awards and honours including CRSI Bronze Medal, IUPAC Young Affiliate, Marie Curie Fellowship, Alexander von Humboldt Fellowship. He is the Editorial Board Member, Nature Scientific Reports. His current research mainly focused on Single molecule/particle spectroscopy-microscopy, Ultrafast-ultraslow dynamics, Semiconductor quantum dots, Perovskites, Meta-fluorophores, Flexible crystals.

Estimating Efficacy of Different Regions of the Solar Spectrum Towards Controlling Exciton Dynamics in Super-Bright, Highly-Pb-Replaced Perovskite Nanocrystal

Abstract: CsPbI3 Perovskite nanocrystal (PNC) absorb the longer range of the solar spectrum than other PNCs such as CsPbCl3 and CsPbBr3 or mixed halide PNCs. CsPbI3 PNC is known to be quite bright [1,2], however, there is a very strong quest to increase the brightness. Brightness = molar extinction coefficient (ε) x PLQY and hence increasing brightness can be approached following two means, i.e. by increasing (i) ε and (ii) PLQY. Till date efforts have been mostly directed towards enhancing PLQY [1,3-6]. Moreover, CsPbI3 PNC contains toxic metal Pb, thereby restricting it towards sustainable applications. Hence, very serious efforts are in place towards achieving super-brightness in highly Pb replaced CsPbI3 PNC [1,3,4]. So far, near unity PLQY for CsPbI3 PNC has been achieved only with <10% Pb replacement in PNCs [1,4]. There is so far no report towards increasing brightness through increasing ε of CsPbI3 or for that matter any PNCs. In the current effort, super-brightness has been achieved in highly-Pb-replaced (as high as 50% Pb replacement) Zn alloyed CsPbI3 PNC, through extremely high values of both ε (1x108 M-1cm-1) and PLQY (98%). Therefore, Zn alloyed CsPbI3 PNC is the most-bright nanomaterial among the PNCs [7-8]/quantum dot family [9-12]. From the applications point of view, it is important to know how different regions of the solar spectrum control the efficacy of the exciton dynamics in case of PNCs. Exciton dynamics in this super-bright highly-Pb-replaced CsPbI3 PNC has been investigated employing (i) fast TCSPC, (ii) ultrafast transient absorption and (iii) ultrasensitive single particle spectroscopic techniques. Fast TCSPC technique based investigation revealed that through Zn-alloying, very significant enhancement of the magnitude of radiative rate constant and reduction in the magnitude of non-radiative rate constant could be achieved. Ultrafast transient absorption technique based investigation revealed that the magnitudes of (a) ultrafast rise time (110 – 750 fs) as well as (b) normalized bleach amplitude (ΔA/A), are dependent on different regions of the solar spectrum. Ultrafast hot exciton trapping dynamics has been observed to be happening in ~1 ps. Ultrasensitive single particle spectroscopy based investigations revealed that the magnitude of truncation time in the probability density distribution of ON events duration is dependent on different regions of the solar spectrum as well.All these very interesting results will be discussed and correlated with each other.

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Invited Speaker

Prof. R Geetha Balakrishna

Jain University,Bangalore

Date: March 2

Time: 2.00PM – 2.30PM

Bio: Prof. Geetha Balakrishna is Director of Centre of Nano and Material Sciences (CNMS) Jain University,Bangalore, Karnataka India. She received her doctoral degree from Bangalore university. She worked as visiting scientist at National university of Singapore, and JNCASR Bangalore. She is recipient of Fulbright fellowship and other numerous awards. Her current research mainly focused on photochemistry and water purification, solar energy and quantum dots, nanoparticles and bioenergy.

Suppression of Phase Segregation and Anion Exchange in Halide Perovskites towards Tandem Photovoltaics

Abstract: Tremendous advances in perovskite solar cells (PSCs) have been achieved in terms of power conversion efficiencies (PCEs), large-area fabrication and device stability since their emergence in 2009, especially after 2012, making PSCs become significant candidates for next-generation photovoltaic technologies. The ease of halide ion exchange in perovskites, with ABX 3 (X=halide) type structure offers convenience to prepare gradient architectures so as to harvest photons in the entire visible region. On the other hand mixed halide perovskites (X= Br/I/Cl) suffer from phase segregation under light irradiation and, studies demonstrate that halide ion defects play a major role in this photo induced halide segregation (PIHS). Several attempts like iodide treatment, interface modulation across electron transport layer/absorber layer and passivation strategies have been implemented previously by our group to supress this PIHS. One such effective approach deploys polyvinylpyrrolidone (PVP) which can substantially suppress PIHS and also reduce anion exchange reactions in gradient perovskite structures. This approach also bestows chemical and photostability to the perovskite in addition to improvement in charge carrier dynamics and thin film quality, the most desired parameters for solar cell devices. This method which can simultaneously suppress anion exchange reaction and PIHS is an important progress in fabrication of photo and chemically stable perovskite thin films as absorbers in tandem photovoltaic devices.

Invited Speaker

Dr Arijit Kumar De

IISER, Mohali

Date: March 2

Time: 2.30PM – 3.00PM

Bio: Prof. Arijit K De is a distinguished Professor at the Dept. of Chemical Sciences, IISER Mohali, Punjab. Prof. Arijit received his doctoral degree from IIT Kanpur. Thereafter, he pursued his post-doctoral research, from Lawrence Berkeley National Laboratory and Dept. of Chemistry, University of California Berkeley, USA. He has received numerous awards including SERB (DST) Early Career Research Award. The principle research interest of Prof. Arijit is Chemical dynamics in condensed phase: Ultrafast spectroscopy and Optical trapping.

Mapping hot carrier relaxation mediated by low-frequency phonon modes in a lead-free double perovskite

Abstract: In this talk, following a brief overview of the research pursued in our group on ultrafast exciton/charge carrier dynamics in perovskites for photovoltaic applications, I will discuss how we can map the time-evolution of low-frequency phonon modes as the hot carriers relax using broadband time-resolved impulsive stimulated Raman scattering (TR-ISRS) recently developed in our group. Specifically, it will be shown how impulsive Raman scattering with spectral dispersion of a chirped broadband probe has many more advantages over conventional (spontaneous or stimulated) Raman scattering.

Invited Speaker

Prof. Janardan Kundu
IISER, Tirupathi

Date: March 2

Time: 3.00PM – 3.30PM

Bio: Prof. Janardan Kundu is a distinguished professor at Department of Chemistry, IISER Tirupati. Prof. Kundu received his doctoral degree in Chemistry from Rice University, Houston, TX, USA, and carried out his postdoctoral research at Center for Integrated Nanotechnologies, Los Alamos National Laboratory, Los Alamos, NM, USA. The principle research interest of Prof. Kundu focuses on semiconductors (bulk and nano materials), metals, and their heterostructures for applications in energy and environment.

Stereochemical Activity of ns2 Metal Ions & Dopants, Structure-Property Correlation, Host-Dopant & Dopant-Dopant Interaction in Low Dimensional Metal Halide Hybrids

Abstract: 3D lead halide perovskite has seen a phenomenal research interest in the last decade for applications in photovoltaics and solid state lighting. Their low dimensional counterparts (2D, 1D, 0D), supporting strongly bound excitons, are well-suited for lighting applications. These low dimensional metal halide hybrids show narrow band edge and broadband self-trapped excitonic (STE) emission. In the absence of general guidelines to enhance this broadband emission, structure-property correlation can be beneficial in designing highly emissive materials. In this talk, I will highlight the fundamental factors that control the emissive properties of main group ns2 metal halide based low dimensional (1D, 0D) hybrids. The mechanism of broad band emission in these low D perovskites, involving STEs and the stereochemical activity of the ns2 lone pair, will be discussed. I will showcase our current results on multi-metallic halide hybrids incorporating hetero-metallic units that manifest interesting photo-physical properties. Effects of electronic interaction between the metal halide units in such multi-metallic low dimensional hybrids will be highlighted. Mechanism of the electronic cross-talk between the isolated metal halide units in such systems will be discussed. I will conclude the talk with outlook of our current research work highlighting the existing issues in white light emission using main group low dimensional metal halide hybrids.

Invited Speaker

Prof. Prof. Zishan Husain Khan

Jamia Millia Islamia, New Delhi

Date: **March 2**

Time: 3.30PM – 4.00PM

Bio: Prof. Zishan Husain Khan is Professor in the Department of Applied Sciences and Humanities, Faculty of Natural Sciences, Jamia Millia Islamia, New Delhi. He obtained his Ph.D. degrees from Jamia Millia Islamia, New Delhi. He went to National Tsing Hua University, Hsinchu, Taiwan for post Doctorate. His present research interests include Nano chalcogenides, Amorphous Semiconductors, Carbonaceous Nanomaterials, Organic Semiconducting Nanostructures and Devices, Nano-sensors, Nano-biosensors and Nanotechnology based optoelectronic devices.

Invited Speaker

Prof. K.V. Adrash
IISER, Bhopal

Date: March 2

Time: 5.45PM – 6.15PM

Bio: Prof. Adarsh is Professor in Department of Physics at IISER Bhopal. He received his Ph.D. in Experimental Condensed Matter Physics from Indian Institute of Science at Bangalore. His research interest focus on Ultrafast effects in semiconductors, optical control of multi-photon absorption, Electro-optic effects, Generation and modulation of Terahertz radiation, Supercontinuum generation in photonic crystal fibres, Quantum size effects and tunability of optical parameters in amorphous semiconductors.

Emergent Correlated Coherent Phenomena in Size and Shape Controlled Metal Halide Perovskite Quantum Dots

Abstract: Many-body interactions of charge carriers in quantum confined semiconducting nanostructures are enhanced relative to their bulk counterparts and thus have opened new opportunities for manipulating and enhancing light-matter interactions. From a fundamental point of view, the enhanced Coulomb interactions due to the low dimensional confinement endow carrier–carrier interactions, predicted to generate exotic correlated effects such as exciton complexes, coherent optical Stark effect, Mott transitions, bandgap renormalization, and condensation of charge carriers. In this talk, I will be discussing the many-body interactions in the semiconducting solution processable metal halide perovskite (MHP) quantum dots (QDs) of the general formula ABX3, the unusual coherent optical Stark effect of redshift, Autler-Townes like splitting and blue shift as a function drive photon frequency in the framework of interacting biexciton picture, spin selective bandgap renormalization, electron-hole liquid at room temperature and low gain threshold for amplified spontaneous emission in size and shape controlled Metal Halide Perovskite Quantum Dots.

Invited Speaker

Dr. Subhendu K. Panda

CSIR-CECRI

Date: March 2

Time: 6.15PM – 6.45PM

Bio: Dr. Subhendu Kumar Panda is a scientist at CSIR-Central Electrochemical Research Institute (CECRI) in Karaikudi, Tamil Nadu, India. He received his doctoral degree from Jadavpur University (Indian Association for the Cultivation of Science, Kolkata). He has received numerous awards and honours including, Alexander von Humboldt Fellow (AvH Foundation), Bhaskara Advanced Solar Energy (BASE) Fellow (DST-IUSSTF) His research interests include Nanoscience and materials chemistry; Colloidal synthesis and studies on photo-physical properties of semiconductor nanostructures; Applications of semiconductor nanomaterials in the field of solar cells, LEDs, Sensors and fuel cells.

Halide Perovskites: Promising Materials for Next Generation Renewable and Sustainable Energy Demands

Abstract: In recent years, halide perovskite materials gaining huge attention due to their excellent optical and electrical properties such as higher absorption coefficient in the visible region and suitable bandgap (1.45 eV-1.60 eV) which lies on the Schottky-Queasier bandgap limit. Tunable bandgap by varying the halide composition. Further, increasing power conversion efficiency (PCE), simple solution fabrication process, light-weight wearable and deployable for ultra-lightweight space and low-cost materials etc. Over the last few years, the efficiency of perovskite solar cells has surpassed 25% due to high-quality perovskite-film accomplished through low-temperature synthesis techniques along with developing suitable interface and electrode-materials. Besides these excellent solar cell properties, these materials showed excellent performance in the luminescence devices such as LEDs and photodetectors etc. Additionally, these materials showed better performance in the water electrolysis through the photoelectrocatalytic water splitting. Recently, ambient atmosphere stabilized photoactive perovskite α-FAPbI 3 and tunable emission properties (warm white light emission to cool white light emission) from the double perovskite Cs 2 InAgCl 6 by the alloying with Na/K and doping with Lanthanides. In this talk, the perovskite material used in the various application such as solar cells, back light white LEDs and PEC water splitting will be discussed.

References:

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Invited Speaker

Prof. Pralay Santra

CSIR-CECRI

Date: **March 2**

Time: **6.45 pm – 7.30 pm**

Bio: Dr. Pralay K. Santra is a Scientist at Centre for Nano and Soft Matter Sciences, Bangalore. He received his doctoral degree from Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore and carried out his postdoctoral research at Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, Department of Chemical Engineering, Stanford University, Stanford, Department of Physics and Astronomy, Uppsala University, Uppsala Subsequently. He received MRSI (Material Research Society of India) Young Scientists' Award. His current research mainly focused on Quantum dot and perovskite photovoltaics, Interfacial recombination, Electron transfer kinetics, Superlattice and Crystallite Orientation in Quantum Dot Solids, Atomic Layer Deposition.

Invited Speaker

Prof. Deepa Khushalani

TIFR

Date: **March 3**

Time: 9.00AM – 9.30AM

Bio: Prof. Deepa Khushalani is a distinguished Professor of Materials Chemistry in the Department of Chemical Sciences at Tata Institute of Fundamental Research (TIFR). Prof. Khushalani received his doctoral degree in Materials Chemistry from University of Toronto, and carried out her postdoctoral research at University of Bristol, UK .The principle research interest of Prof. Khushalani involves materials chemistry with emphasis on exploiting inorganic structures in devices catering to alternate sources of clean energy involving photovolatics and energy storage devices.

Low Dimensional Hybrid Perovskites

Abstract: In terms of effectively exploiting solar energy, one option is to approach this problem as converting solar energy to an electrical impulse using solar cells. Over the last ca. 15 years that there has been an exponential increase in the interest shown on light absorbing hybrid perovskite based solar cells. However, despite all enormously impressive advantages of MAPI (methyal ammonium lead iodide), one aspect that has frustrated researchers is the lack of temporal and thermal stability of this material. Towards solving this issues, several approaches have been tried however, one major development that has stood-out is the incorporation of different cations in the A-site and different halides in the B-site. This compositional mixing with the perovskite stoichiometry has not only exerted a strong influence on efficiency but most importantly also raised the stability substantially. Hybrid perovskites with mixed cation and anion compositions can be tailored to optimize specific properties, such as bandgap and absorption coefficient, improving carrier dynamics and mitigating ion migration for applications in solar cells and other optoelectronic devices. In this presentation, I will showcase our foray into the synthesis of single crystalline and thin films of mixed ion hybrid perovskites. I will discuss both 3D and 1D systems and the ensuing characterisation will be detailed involving structural and opto-electronic properties.

Invited Speaker

Dr. Vinod Erkkara Madhavan

NIT, Calicut

Date: March 3
Time: 9.30AM – 10.15AM

Bio: Prof. Vinod E. Madhavan is a professor at School of Materials Science & Engineering, NIT Calicut, Kerala, India. He received his doctoral degree from Indian Institute of Science, Bangalore and carried out his postdoctoral research at IISc Bangalore.

Inorganic Hole Transport Material with 3D/2D Perovskite Solar Cells for higher stability

Abstract: The stability of perovskite solar cells (PSC) can be improved by combining passivation and protection techniques, which involve using a thin layer of 2D perovskite and inorganic HTM, respectively. In this study, we have found that adding a thin layer of (Phenylethyl)ammonium (PEA) or [(4-fluorophenyl)ethyl]ammonium (FPEA) 2D perovskite on top of the 3D perovskite absorber layer can enhance device stability while maintaining a moderately high power conversion efficiency. This approach neutralizes defects on the surface of the 3D perovskite absorber, providing protection against moisture-induced degradation. Additionally, the modified interfaces show excellent charge extraction into the inorganic CuSCN HTM, with device efficiencies above 18%. The use of 2D perovskites and CuSCN as an innovative device architecture significantly improves the stability of PSC, as evidenced by the results of aging tests which show a slowing down of degradation even after 1 year. Theoretical calculations using drift-diffusion simulations support these findings, indicating that a thin layer of a wide band gap has only a minor influence on the device efficiency.

Invited Speaker

Prof. Supravat Karak

IIT, Delhi

Date: **March 3**

Time: 10.15AM – 10.45AM

Bio: Prof. Supravat Karak is a distinguished Professor at the Department of Energy Science and Engineering, IIT Delhi. Prof. Karak received his doctoral degree in physics from IIT Kharagpur. Thereafter, he pursued his post-doctoral research from University of Massachusetts, USA. He has also worked with Prof.KunioAwaga at Nagoya University as a JSPS fellow. He has received numerous awards including Early Career Research Award, SERB-DST. Prof. Karak group is focused broadly on the fundamental opto-electronic properties of organic and hybrid semiconductors for photovoltaic applications. Fabrication of organic and hybrid molecule based photovoltaic devices and understanding the fundamental photo-physics of new class of material systems to improve their performance both in terms of efficiency and lifetime, and ultrafast THz photodetectors are his primary research interests.t IISc Bangalore.

Inorganic Hole Transport Material with 3D/2D Perovskite Solar Cells for higher stability

Abstract: The stability of perovskite solar cells (PSC) can be improved by combining passivation and protection techniques, which involve using a thin layer of 2D perovskite and inorganic HTM, respectively. In this study, we have found that adding a thin layer of (Phenylethyl)ammonium (PEA) or [(4-fluorophenyl)ethyl]ammonium (FPEA) 2D perovskite on top of the 3D perovskite absorber layer can enhance device stability while maintaining a moderately high power conversion efficiency. This approach neutralizes defects on the surface of the 3D perovskite absorber, providing protection against moisture-induced degradation. Additionally, the modified interfaces show excellent charge extraction into the inorganic CuSCN HTM, with device efficiencies above 18%. The use of 2D perovskites and CuSCN as an innovative device architecture significantly improves the stability of PSC, as evidenced by the results of aging tests which show a slowing down of degradation even after 1 year. Theoretical calculations using drift-diffusion simulations support these findings, indicating that a thin layer of a wide band gap has only a minor influence on the device efficiency.

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Invited Speaker

Prof. Ganapathy Veerappan
ARCI

Date: March 3

Time: 10.45AM – 11.00AM

Bio: Prof. Ganapathy Veerappan is a scientist at ARCI. Prof. Ganapathy received his doctoral degree in Chemical Engineering from Pohang University of Science and Engineering, and carried out his postdoctoral research at Sungkyunkwan University (SKKU), South Korea. The principle research interest of Prof. Ganapathy is Perovskite Solid state solar cells, Organic-Inorganic Heterojunction solar cells & Organic solar cells, Dye-sensitized solar cells.

Carbon based Perovskite Solar Cells for Scalability and Stability

Abstract: At present, the total electricity produced is not enough to meet the global energy demands. Tens of giga-watts of wind turbines, hydropower generators and solar photovoltaic modules are installed worldwide. It is anticipated in the future that about one-thirds of the energy generated would be from solar photovoltaics (PV) technology. Of all the renewable energies available, solar PV is dominant with an annual growth rate of 60% between 2000 and 2016. After a decade of research in perovskite solar cells (PSCs) researchers all over the world are aiming for large area PSCs with real-time applications. But utilization of noble metal cathode and organic hole transporting material causes serious concerns in device instability, scalability and processing cost. Carbon based PSCs (CPSCs) were introduced to overcome these shortcomings. In this talk, we will highlight some of the important findings of our group's research in carbon based and conventional PSCs and its future perspective.

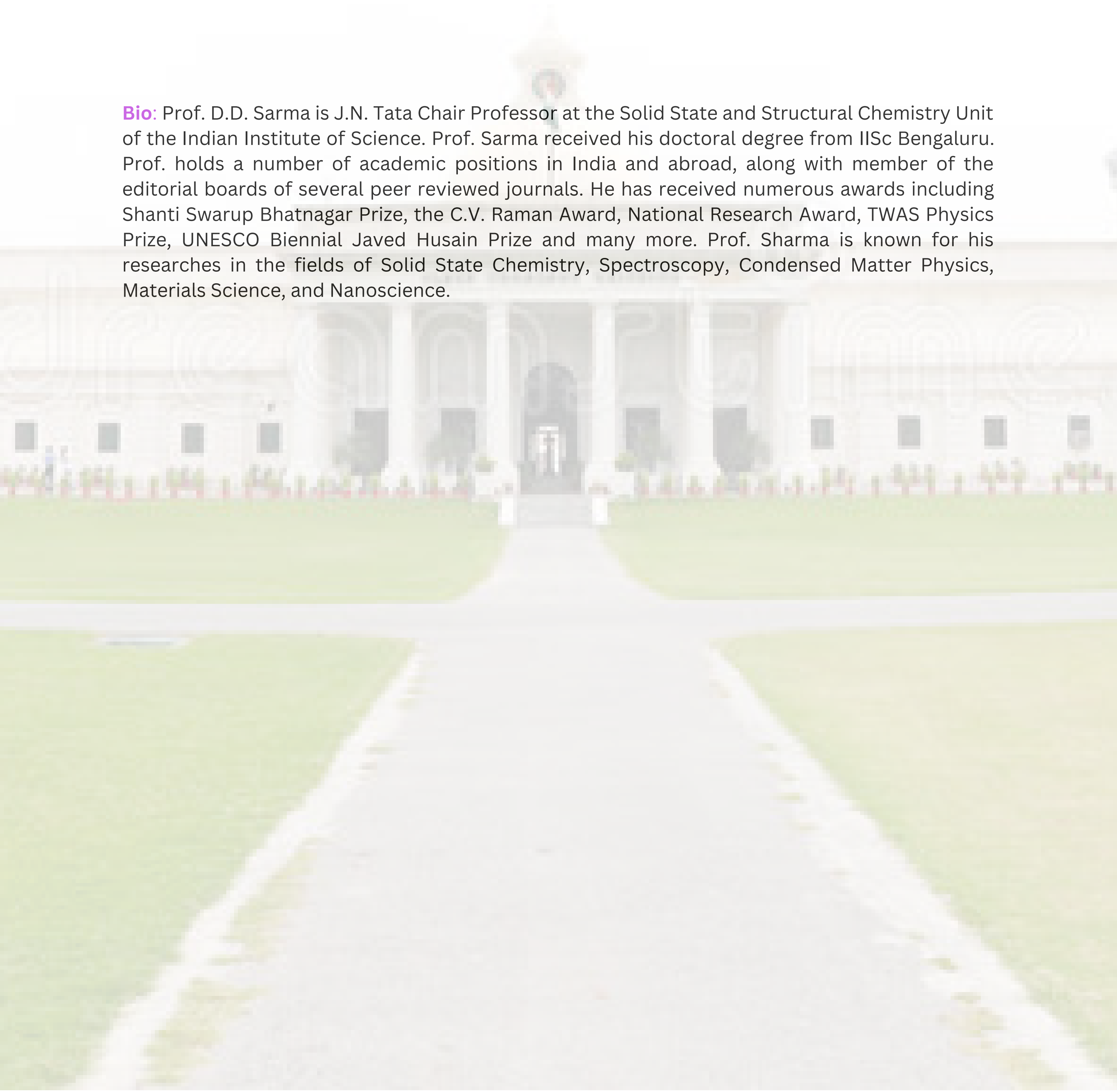
Invited Speaker

Prof. D. D. Sarma

IISc

Date: **March 3**

Time: **11.30AM – 12.00PM**



Bio: Prof. D.D. Sarma is J.N. Tata Chair Professor at the Solid State and Structural Chemistry Unit of the Indian Institute of Science. Prof. Sarma received his doctoral degree from IISc Bengaluru. Prof. holds a number of academic positions in India and abroad, along with member of the editorial boards of several peer reviewed journals. He has received numerous awards including Shanti Swarup Bhatnagar Prize, the C.V. Raman Award, National Research Award, TWAS Physics Prize, UNESCO Biennial Javed Husain Prize and many more. Prof. Sharma is known for his researches in the fields of Solid State Chemistry, Spectroscopy, Condensed Matter Physics, Materials Science, and Nanoscience.

Invited Speaker

Prof. Rupak Banerjee

IIT, Gandhinagar

Date: March 3

Time: 12.00PM – 12.30AM

Bio: Prof. Rupak Bannerjee is a distinguished professor of Physics at Indian Institute of Technology, Gandhinagar. Prof. Bannerjee received his doctoral degree from University of Calcutta (Saha Institute of Nuclear Physics). The principle research interest of Prof. Bannerjee focuses on understanding the growth mechanisms and applications of various organic, inorganic, and hybrid-material thin-films, and nanomaterials.

Mechanism of Ionic Conductivity, Dielectric Relaxation, and Energy Harvesting Properties of Halide Perovskites

Abstract: We study the dielectric, piezoelectric, and ferroelectric properties of halide perovskites over a wide temperature and frequency range. By analyzing the dielectric data in terms of complex impedance spectroscopy, AC conductivity, and complex electric modulus using the Maxwell-Wagner equivalent circuit model, the universal Universal Power law, the Havrilliak-Negami, and the Kohlrausch-Williams-Watts models, the fundamental aspects of the transport and relaxation mechanism in perovskites are unraveled. The contribution of the grains and grain boundaries to the overall impedance spectroscopy could be understood by the Nyquist plots. A temperature region is observed, where the DC conductivity is almost constant, but the DC conductivity increases both below and above this region. We identify this region as the phase transition region where the ferroelectric to paraelectric phase transition occurs. We note that the conduction mechanism changes from overlapped large polaron tunneling to correlated barrier hopping due to the ferroelectric to the paraelectric phase transition. The activation energy derived from experiments matches the theoretical models. The material exhibits decent saturation polarization and a large piezoelectric constant. We fabricate composites of perovskites with polyvinylidene fluoride (PVDF) with varying weight percentages of perovskite in the PVDF matrix to assess their energy-harvesting performances.

Keywords: Halide perovskites, Dielectric spectroscopy, Activation energy, Ferroelectricity, Piezoelectric nanogenerator

Invited Speaker

Prof. Pankaj Yadav

PDEU

Date: **March 3**

Time: 12.30AM – 1.00PM

Bio: Prof. Pankaj Yadav is a distinguished Professor at Pandit Deendayal Petroleum University (PDPU), Gujarat, India. Prof. Yadav received his doctoral degree in Photovoltaic Science and Engineering from Pandit Deendayal Petroleum University, and carried out his postdoctoral research at Incheon national University (South Korea). Dr. Yadav is a recipient of many prestigious awards including Fulbright fellowship, Swiss Excellence fellowship, etc. His current research interests ranges from thin film devices, solar photovoltaic, perovskite solar cells, hydrogen generation, fuel cells, energy generation and storage devices, and electroanalytical characterizations.

Invited Speaker

Prof. Shahab Ahmad

IIT Jodhpur

Date: March 3

Time: 12.00PM – 12.30AM

Bio: Prof. Shahab Ahmed is Professor in Computer, Electrical, Mathematical Sciences, and Engineering (CEMSE) Division and ANPERC member at KAUST, Saudi Arabia. Prof. Ahmed received his doctoral degree from Texas A&M University, Texas, USA and worked at Department of Electrical & Computer Engineering, Texas A&M University at Qatar, Doha, Qatar. Professor Ahmed's research interests span the broad areas of power conversion and mechatronic systems. His research aims to intelligently merge electronics/mechanics/computing/control disciplines to develop novel devices and software that serve future smart grids and intelligent oil fields.

Metal Halide Perovskites: From Optoelectronic to Optoionic Devices

Abstract: In the recent past, organometal halide perovskites have gained huge attention for application in various optoelectronic devices such as photovoltaics, light-emitting diodes (LEDs), photo- detectors, lasers, etc. which is attributed to the extraordinary properties of these solution processible semiconductors. 1-2 On the other hand, with several recent advancements in rechargeable battery technology the new generation energy storage systems are comprised of electrodes with multi-functionalities for unconventional applications. For instance, the emerging autonomous electronics, such as IoT devices, require increasingly compact energy harvesting and storage solutions. 3-5 Merging these two functionalities in a single device would significantly increase their volumetric performance. In my presentation, I will discuss about the RP metal halide perovskites based optoelectronic and emerging hybrid photo-rechargeable energy storage devices, where the functionality of the rechargeable battery and the solar cell are merged together in a single device to avail the advantages of both technologies simultaneously. These photo-rechargeable energy storage devices harvest solar energy and stores it in the form of chemical energy, therefore the performance of these devices relies on optoelectronic as well as structural properties of the photoactive materials which enable them to simultaneously achieve photocharging and store metal-ions in a single active material medium.6-8

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Poster Abstracts

Steady-State Analysis of Traps in Perovskite Solar Cells using the Variations in Diffusion-to-Drift Transition Voltage

Abdul Basit Andrabi [1*], Arun Tej Mallajosyula[1].
*Lead presenter
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[1]Department of Electronics and Electrical Engineering,
Indian institute of Technology Guwahati,
Assam, 781039, India.

Abstract: Perovskites contain significant amount of localized states (traps) because of grain boundaries and defects. These traps cause accumulation of space charge near injecting contacts, due to which there is band bending in the vicinity of contacts. This results in a decrease in the transition voltage (V_α), which is the voltage at which the steady-state current changes from diffusion to drift. By examining the V_α of a two terminal perovskite device, we suggest a method to qualitatively study the trap distribution. The validity of this technique has been verified from the numerical simulations carried out using Sentaurus TCAD. Both density (N_T) and energetic depth (E_T) of traps were varied to examine their effect on V_α and on energy bands. Devices with deeper and higher N_T have been found to exhibit stronger band bending and lower V_α. In addition, V_α has been found to be sensitive to N_T even when band bending due to accumulated ions or uncompensated dopants near interfaces is significant. This dependence was further illustrated for a multi-layer solar cell device. The availability of different methods to extract V_α from $J-V$ characteristics, and the extra sensitivity of V_α to N_T paves a way to study traps effectively.

Keywords: Traps, built-in voltage, perovskite, band bending, transition voltage

Ruthenium Halide Double Perovskites and their application in Solar Water Oxidation

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[2] *Centre for Photo- and Electro-Chemical Energy (C-PEC), Institute of Technology Madras Adyar, Chennai, Tamil Nadu 600036, India*

Abstract: Hydrogen is intended as the "holy grail" for the energy community. Solar-water splitting is one of the most promising strategies for producing hydrogen. The abundance of water and solar energy enables the potential of scaling-up up this new technology if suitable photo-electrocatalysts and solar cells are developed. The aqueous stability photo absorbers are essential for developing successful photoelectrochemical (PEC) solar fuel devices. The fascinating optoelectronic properties and chemical tunability of halide perovskites have drawn considerable curiosity. However, their stability in aqueous electrolyte media is poor. The vacancy-ordered double perovskite Cs_2RuX_6 (X = Cl, Br) described here exhibits wizard stability in ambient and aqueous media at extreme pH values (pH 1 to 13). These materials exhibit magnificent absorption properties covering most of the visible spectrum. These ultra-stable materials allow the tuning of optical properties across mixed halide sites. The electrochemical properties of these materials are investigated, showing solar water oxidation on an unprotected photoanode with a photocurrent density of >0.2 mA cm^{-2} at 1.23 V (vs. RHE) under simulated AM1.5G sunlight. These materials show PEC stability for hours without compromising performance in constant voltage measurements.

Keywords: halide perovskites; photoelectrochemical water oxidation; stability; vacancy ordered double perovskites; water splitting.

Fabrication and Simulation of Hybrid Perovskite-based Multilayer Light-Emitting Diodes

Abinash Baruah [1*] and Dr. Arun Tej Mallajosyula
*Lead presenter and Corresponding author
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[1]Department of Electronics and Electrical Engineering
Indian Institute of Technology Guwahati,
Assam, 781039, India

Abstract: Multilayer Perovskite light-emitting diode (PeLED) with MAPbBr3 as an emissive layer has been fabricated and characterized. These devices show a promising luminance of 5409 cd/m2 with a turn-on voltage of 3.8 V and a full width at half maximum (FWHM) of 22 nm. The same Peled device structure has been simulated using 2D SILVACO Technology Computer-Aided Design (TCAD). The simulation considers bipolar carrier transport by Drift-Diffusion mechanism, field-dependent mobilities, bimolecular Langevin recombination model, interface defects, recombination at interfaces, and singlet exciton diffusion effects. Further optimization of the device structure is attempted through simulation using different hole transport layers and electron transport layers for better carrier injection.

Keywords: Perovskite light emitting diode,PeLED, Atlas, Silvaco TCAD.

Fluoroperovskite based down-conversion nanophosphors for enhancing the current density of perovskite solar cells

Acchutharaman K R, [1*] Joel Kingston R,[1] Santhosh N,[1] Balagowtham N,[1] Akanksha Choubey,[1] Senthil Pandian M,[1] Ramasamy P,[1]
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[1]Department of Physics, Sri Sivasubramaniya Nadar College of Engineering, Kalavakkam – 603110, Tamilnadu, India.

Abstract:

Recently, innovative research has been intensively employed on perovskite solar cells (PSCs) to expand their frontiers further. This work is also one such successful attempt to drive the limit of photocurrent density beyond the conventional PSC (which typically utilizing the visible spectrum alone) through a phenomenon called down-conversion (DC). The use of DC luminescence to harness the UV region from the solar spectrum has been explored with an approach by utilizing Eu^{3+} activated $RbCaF_3$, a fluoroperovskite-based phosphor material. It is observed that the $RbCaF_3:Eu^{3+}$ incorporated TiO_2 electron transport layer (ETL)-based PSCs enhanced their photocurrent density as well as UV stability, compared to the PSCs with pristine TiO_2-oriented ETL. Such improvement in the earlier mentioned devices was due to the result of converting high-energy UV photon to effectively absorbable low-energy visible photons for the perovskite absorber. Overall, the DC-aided PSC offered a substantial photocurrent density of 23.54 mA/cm^2 and boosted its power conversion efficiency from 11.2% to 13.3%.

Keywords: down-conversion, photocurrent density, fluoroperovskite, carbon electrode.

Surface treatment of $CsPbIBr_2$ for Processing of Efficient Perovskite Solar Cells

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Tamil Nadu- 603110.

Abstract: Inorganic perovskite solar cells (IPSC) based on $CsPbIBr_2$ perovskite have piqued large interest of researchers because of its upgraded environmental stability, and well-balanced band-gap. Perhaps, to obtain a high-performing perovskite solar cell, it is crucial to improve the interfacial contact between the perovskite layer and adjacent charge transport layers. In this research, we have a modulated the interface between $CsPbIBr_2$ perovskite layer and carbon-electrode with the help of a novel deep eutectic solvent (DES) for manufacturing an efficient and stable carbon-based IPSC. The surface of $CsPbIBr_2$ absorber layer has been passivated with DES to enhance morphology and crystallinity of the film with reduced trap-states at the grain boundaries, thus improving its opto-electronic properties. The energy difference between the perovskite layer and carbon-electrode has been minimized through DES passivating agent which resulted in remarkable increase in the photovoltage of the device. As a result, the efficiency of DES modified device is increased upto 7.02 % in contrast to efficiency (4.75%) of pristine device. The champion device is more resistant to moisture and has been optimized for ambient-air processing of the perovskite solar cells. It shows enhanced thermal stability of over 10 days at 100 °C. Thus, this strategy can open a new and facile way for boasting the performance of C-IPSCs.

Keywords: Inorganic perovskite solar cells, interfacial passivation, passivating agent, ambient-air, and thermal stability.

Revealing the Carrier Dynamics in Perovskite/MoS_2 Heterostructure

Amit kumar Chaudhary[1,2], Naveen Kumar Tailor[3] , Prince Sharma[1,2], Archana Rana[1,2] , Soumitra Satapathi[3] and Mahesh kumar[1,2]

[1] CSIR-National Physical Laboratory, Dr. K.S. Krishnan Marg, New Delhi 110012, India
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ABSTRACT:

Perovskite/2D material heterostructures have emerged as a promising class of materials for optoelectronic applications.Halide perovskite/2D materials heterostructures have made significant strides and show great promise, but there are still a number of research gaps that need to be filled before their potential for real-world applications can be completely realised. The incomplete understanding of the charge carrier dynamics in these hybrid systems is one of the main research gaps in halide perovskite/2D materials heterostructures. In this work, we have revealed the insights into charge carrier dynamics in $CsPbBr_3/MoS_2$ heterostructure using ultrafast transient absorption spectroscopy. We have observed shift in the bands in the case of $CsPbBr_3/MoS_2$heterostructure, which is attributed to modulation of energy levels and interfacial effect between $CsPbBr_3$ and MoS_2. Additionally, we observed that polaronic features are suppressed in heterostructure. Our results provide new insights into the charge transfer dynamics in perovskite/2D material heterostructures which have important implications for the design and optimization of perovskite/2D material heterostructures for a wide range of applications.

Keywords: - *Perovskite, Molybdenum disulfide , Hetrostructure and Ultrafast transient absorption spectroscopy*

Micro-strain management of ZnO/$CH_3NH_3PbI_3$ interface via incorporation of Fullerene (C_{60})

Anand Pandey[#], Lokendra Kumar
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Charge transport layers play a vital role to decide the stability, charge collection, and photovoltaic device parameters of perovskite solar cells. Electron transport layers such as ZnO, TiO_2, and SnO_2, *etc* are currently employed in designing perovskite solar cells. Despite ZnO having superior optoelectronic properties to these metal oxides, such as improved transmittance, higher conductivity, and closer conduction band alignment to methylammonium lead iodide perovskite ($MAPbI_3$), ZnO is unnoticed due to a chemical instability when in contact with metal halide perovskites, which decompose the perovskite. In this work, we have modified the ZnO layer by incorporating fullerene (C_{60}) in different ratios and studying the impact of C_{60} on the ZnO/$MAPbI_3$ interface. The $MAPbI_3$ films were fabricated onto ZnO substrates using a two-step spin coating technique. Lattice strain has been observed and found to be reduced on increasing the C_{60} concentration and at a particular concentration of C_{60}, micro-strain has been altered from tensile strain to compressive strain. Furthermore, Urbach energy and trap levels have significantly reduced due to the incorporation of C_{60} into ZnO films which suggests that the incorporation of C_{60} facilitates the superior optoelectronic feature of perovskite semiconductors.

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Synthesis of Lead-Free Double Perovskite With Great Stability and Opto-Electronic Properties

Anupam Chetia,[1*] Atanu Betal,[1] Satyajit Sahu[1]
*Lead presenter
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[1] *Department of Physics, Indian Institute of Technology Jodhpur, Jodhpur 342037, India*

Abstract: Halide perovskites have gained great interest in the field of optoelectronic applications owing to their excellent optical and electronic properties. Despite having great properties, the stability and toxicity issues are concerns of researchers. In this regard, lead-free double halide perovskite (DHP) materials are the potential candidates to be used in optoelectronic applications. Different works are going on based on lead-free, inorganic, high stable double perovskite, although more study is required to get better result¬. From the above motivation, we have synthesized a highly stable, lead-free DHP $Cs_2CuBiBr_6$ using a simple solution-processed method. XRD and Raman spectroscopy studies were performed and confirmed the successful synthesis of the material in the cubic phase. The optical properties of the materials were studied by UV-Visible spectrophotometer and photoluminescence spectrometer, and we have found the band gap of the materials from the Tauc plot. We have also studied the FE-SEM characterization of the film.

Keywords: **Double perovskite , Highly stable , Non-toxic**

Recovery of Colloidal Ruddlesden-Popper Perovskite Nanoplate: A Curious Case of Thiol

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Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur – 208 016, Uttar Pradesh, India.

Abstract: Quantum confined and moisture stable Ruddlesden Popper (RP) type two-dimensional (2D) perovskite nanoplate (NPl) shows superior performance in the optoelectronics field. But this layered perovskite material also suffers from external perturbations like heat, solvent polarity and specially light irradiation cause the degradation of the parent structure which limits their performance. To extend the understanding on colloidal RP nanoplate, our previous report discussed the transformation of colloidal RP NPl, $(OAm)_2(CH_3NH_3PbI_3)_2PbI_4$ into 3D $CH_3NH_3PbI_3$ nanorod (NR) structure under 365 nm UV exposure. In this contribution, we have systematically studied the fate of UV exposure on the same colloidal RP NPl which is sufficiently dilute (30 times, D30) and the result is degradation instead of transformation. Here for the first time we are successful to recover the parent colloidal RP perovskite structure by organic thiol molecule from its UV degraded stage. First, we have systematically studied the UV assisted degradation of colloidal NPl and isolated degradation products in different stage. The deprotonation of alkylammonium ion in presence of UV light and oxygen causes for this structural degradation. From the acquired knowledge of degradation mechanism, we added proton donating organic thiol in one of the degradation stages and recovered total structural integrity with photoluminescence.

Keywords: Colloidal Ruddlesden Popper Perovskite, UV assisted degradation, recovery, organic thiol, deprotonation-protonation

Layered Halide Perovskite Thin Film for Pollutant Detection and Nonconventional Photocatalytic Degradation

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Department of Chemistry, Indian Institute of Technology Bhilai, Chhattisgarh, 492015

Abstract: 2D-LHaPs (Layered halide perovskites), with a structural formula of R_2PbX_4; R= organic spacer containing long chain aromatic amine and X= halide, offers better ambient stability compared to 3D-HaPs. The potential of 2D-LHaP thin film towards the visible-light-driven photocatalytic degradation of toxic 2-mercaptobenzothiazole(MBT) was examined in hexane medium. Optoelectronics of the 2D-LHaP were investigated as a function of the 'X' site. The thermal stability of the synthesized 2D-LHaP thin films was also examined by thermogravimetric analysis and temperature-dependent XRD. During the photocatalysis experiment, the rate constants of the thin films were calculated with a value of $3\text{-}6\times10^{-2}$ min^{-1}, under visible light illumination. Cycling experiments were performed with the thin films to understand their behavior under repeated runs. Faster rate kinetics was observed when the Perovskite was coated over the titanium dioxide, indicating hole-dominated degradation. The same concept was proved using chronoamperometric analysis. Less toxic MBTS product was suggested by mass spectrometric analysis, via most probable $^{\cdot}O_2$ radicals mediated degradation. The adsorption of MBT over the 2D-LHaP was also 'detected' using photoluminescence analysis. Thus, 2D-LHaP thin films exhibited a promising photocatalytic action, to the prospect of "detection and degradation" of harmful contaminants.

Keywords: Layered Halide Perovskite; Two-dimensional materials; Ambient Stability; Photocatalysis; Photo-electro-chemistry.

Partially Oxidized Metal as Carrier Selective Electrode in Substrate Configuration Perovskite Solar Cells

Arun Kumar [1*], Sonia Rani[1], Dhriti Sundar Ghosh[1,2]

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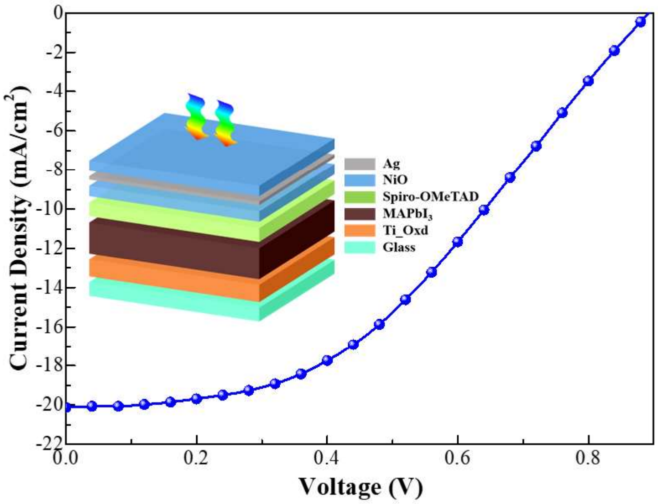
[2]Department of Physics, Indian Institute of Technology (IIT) Dharwad, Dharwad, India

Abstract: Fabrication of photovoltaic devices over metallic films can enable easy integration of photovoltaic technology with vehicles, gadgets, buildings, etc. Herein, a vapor-deposited thick titanium (Ti) film has been utilized as a bottom metal contact for the fabrication of planar perovskite solar cell (PvSC) under the p-i-n configuration. Partial oxidation of Ti film via thermal treatment can help to make it an electron-selective contact, without employing any additional carrier-selective transport layer. An indium-free oxide-metal-oxide based NiO/Ag/NiO (NAN) is used as the top transparent electrode (TE) enabling the illumination of the photoactive layer. A planar device with architecture Glass/Ti_Oxd/MAPI/Spiro-OMeTAD/NAN has been realized and a power conversion efficiency (PCE) of 7.6% was obtained with an active area of 0.25 cm^2. The fabricated devices (without encapsulation) were found to be stable under ambient environmental conditions and retain over 80% of their initial PCE over 500 hours. The highly reproducible, temperature-compatible, and low-cost technique can help in the large-scale fabrication of photovoltaic devices and their integration with gadgets and automobile technologies.



Keywords: Perovskite Solar Cells, Substrate Configuration, Carrier Selective Electrode, Transparent Electrode, Oxidized Metal.

Photocurrent Maximization and Energy Density Calculation of All-Perovskite Tandem Solar Cells

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Abstract:

Three optimization algorithms, all based on the transfer matrix method (TMM), have been developed and validated for the optical modelling of 2T tandem solar cells (TSCs). These algorithms have been compared when applied to organic-inorganic hybrid perovskite (OIHP) based TSCs. The thicknesses of active perovskite layers and different interlayers, including metals and transparent conducting oxides (TCOs), have been optimized for maximizing the device efficiency. Dependence of photocurrent density (J_{PH}) on the angle of light incidence has been estimated for this TSC. To calculate the maximum amount of energy that these TSCs can generate in an year, the energy densities generated per day were integrated and compared using the solar irradiation and temperature data for our institute location from PVGIS-SARAH, European Commission database. Despite generating the highest short circuit current density at normal incidence, the Ag-interlayer TSC generates 79% and 82% lower energy density than these TSCs on the longest day of the year. Among all the interlayers studied here, Ti and ITO have been found to be the best metal and TCO respectively. These findings could be helpful in the performance assessment and development of lead-free all-perovskite TSCs in the near future.

Keywords: Transfer matrix method, Energy density, Organic inorganic hybrid perovskite, Tandem solar cell, Interlayer

Study of Carbon Dioxide Sensing Characteristics of Barium Titanate Perovskite

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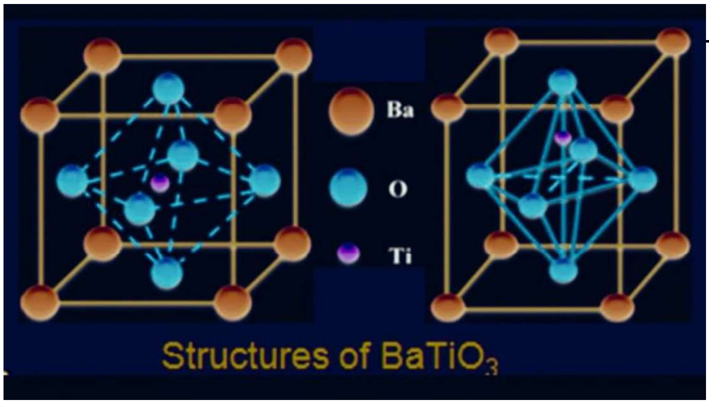
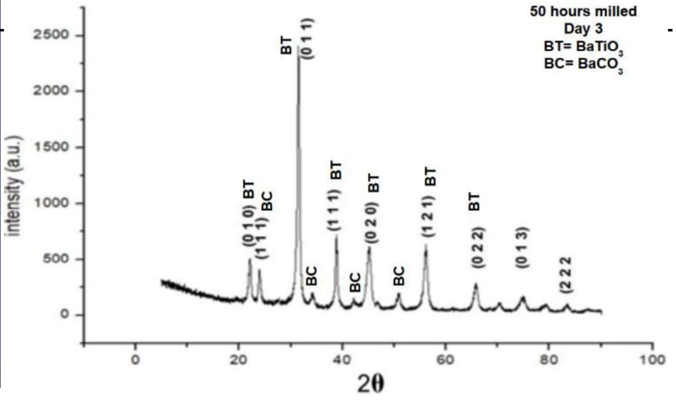
Abstract:

Barium titanate ceramic is one of the technologically important ferroelectric material and widely used in electronic industries for the multi layer ceramic capacitor (MLCC). Now-a- days, size effect on the dielectric properties of $BaTiO_3$ perovskite is receiving exraordinary importance due to the miniaturization of electronics devices. The technological trend towards decreasing dimension makes it of interest to examine its functional properties at nano-scale. Mechanical milling is the easiest and cheapest method to prepare the nano materials from bulk materials. It has been observed that nano-structured BaTiO3 reacts with atmospheric carbon dioxide to form $BaCO_3$ at nano-scale. The advantage of this process lies in the fact that effect of milling hours, reduction in particle size and the lattice strain imparted to them, bear direct relation with the rate as well as the quantity of absorbed CO_2 . Thus, this particular process can be considered better off to study the sensing characteristics of these nanoparticles because enormous scope of selectivity, an essential requirement for sensing applications, are available among aforesaid parameters of particle size, lattice strain, gas absorption rate etc. The present work will be discussed regarding Carbon dioxide sensing characteristics of nanocrystalline $BaTiO_3$ and its effects on the structural and dielectric properties of nanocrystalline $BaTiO_3$.





Development of Ultra-High Sensitivity Spectroscopic Techniques

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Abstract: I will be discussing about the development of two ultra-high sensitive absorption spectroscopic techniques, namely, PDS (Photo-thermal Absorption Spectroscopy) and FTPS (Fourier Transform Photo-current Spectroscopy). Both of them are used for material characterization (specially Perovskite and many more) across the globe. PDS is an optical method whereas FTPS is an electrical one. These techniques offer crucial insights that can play a critical role in achieving/optimizing perovskite device fabrication to result in high power conversion efficiencies.

With the help of PDS, we can achieve up to 5-6 orders of dynamic range of sensitivity, where, with FTPS, we can reach even up to 9-10 orders. This will help us in understanding of sub-bandgap absorption originating from deep level defect/trap states which are otherwise impossible to encounter through normal absorption spectroscopic techniques (namely, UV-Vis).

I will be discussing about the development of the PDS and FTPS and also shine light on the challenges that one encounters along with the ways out.

Keywords: Spectroscopy, Defects, Urbach Energy, Perovskite solar cells

Facets-Directed Epitaxially Grown Lead Halide Perovskite-Sulfobromide Nanocrystal Heterostructures and Their Improved Photocatalytic Activity

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Abstract Lead halide perovskite nanocrystal heterostructures have been extensively studied in the recent past for improving their photogenerated charge carriers' mobility. However, most of such heterostructures are formed with random connections without having strong evidence of epitaxial relation. Perovskite-chalcohalides are the first in this category, where all-inorganic heterostructures are formed with epitaxial growth. Going beyond one facet, herein, different polyhedral nanocrystals of $CsPbBr_3$ are explored for facet-selective secondary epitaxial sulfobromide growths. Following a decoupled synthesis process, the heterojunctions are selectively established along {110} as well as {200} facets of 26-faceted rhombicuboctahedrons, the {110} facets of armed hexapods, and the {002} facets of 12-faceted dodecahedron nanocrystals of orthorhombic $CsPbBr_3$ which have been extensively studied with electron microscopic imaging. Unfortunately, these heterostructures did not retain the intense host emission because of their indirect band structures, but such pseudo-Type-II combinations are found to be ideal for promoting photocatalytic CO_2 reduction and improving their catalytic activities.

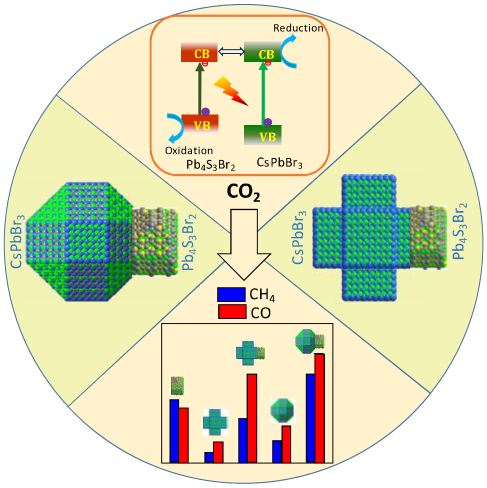

Fig.1. Epitaxially Grown Lead Halide Perovskite-Sulfobromide Heterostructures and Their Improved Photocatalytic Activity

Keywords: Lead Halide Perovskite, Sulfobromide, Heterostructures, Epitaxial Connection, Photocatalysis.

Unveiling the Temperature-Dependent Carrier Relaxation Processes in $CsPbCl_3$ Perovskite Nanocrystals

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Inorganic Lead halides Perovskites have been gaining massive consideration in the field of optoelectronics as an emerging material with great potential to develop high-end optoelectronics. Cesium lead chloride ($CsPbCl_3$) has been under constant consideration for its capability to emit blue light and has the potential to be doped or stacked with another complementary material.[1] Though, it undergoes subsequent temperature-dependent phase transition which is one of the vital physical phenomena in solid-state physics. Still, the association between the carrier relaxation processes and the structural phase transition of $CsPbCl_3$ is unknown. In this current investigation, the temperature as well as excitation energy-dependent fundamental photo physics in $CsPbCl_3$ have been profoundly explored by engaging ultrafast transient absorption and terahertz spectroscopy. The carrier relaxation, carrier temperature, and energy loss portray a direct dependence on the phase transition exhibited by the nanocrystals. Further, to understand excitation energy dependence over photoconductivity and mobility the optical pump THz probe measurements were conducted and it is instituted that the mobility decay slows down as excitation energy is reduced. Overall, the inferences drawn from our study render $CsPbCl_3$ a fascinating material to understand the behavior of carriers upon phase transition and excitation energy.

Keywords: *low temperature, phase transition, perovskite, carrier temperature, mobility*

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Investigation of the photovoltaic performance of lead-free vacancy-ordered Double Perovskite Cs_2SnI_6 using DFT and SCAPS-1D Simulation Approaches

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Abstract: The electrical and optical characteristics of the absorber layer have a significant impact on the efficiency of a perovskite solar cell. Quantum mechanical technique, such as first-principles calculation within density functional theory (DFT) framework, is required for high-precision predictions for optoelectronic characteristics of PSC absorber layers. We first calculated the structural, electronic, and optical characteristics of the proposed double perovskite Cs_2SnI_6 using the DFT-method through Wien2k software with the help of TB-mBJ potential function. The band gap of Cs_2SnI_6 is to found out to be 1.13 eV. The SCAPS-1D programme is used to model the n-i-p structure (Glass/ITO/TiO_2/Cs_2SnI_6/PEDOT: PSS/Au), utilizing the DFT-extracted band gap, carrier mobility, and absorption coefficient spectra during simulation. Indium-doped tin oxide (ITO) and gold (Au) were used as front and back contacts respectively. Titanium dioxide (TiO_2) and Poly(3,4ethylenedioxythiophene)-polystyrene sulfonate) PEDOT: PSS are used as an electron transport layer (ETL) and organic hole transport layer (HTL) respectively, while caesium tin iodide double perovskite (Cs_2SnI_6) is used as the absorber layer. The simulated perovskite solar cell exhibited outstanding performance with a power conversion efficiency (PCE) of 20.23 %, a fill factor (FF) of 70.40 %, an open circuit voltage (V_{oc}) of 0.72 V, and a short circuit current (J_{sc}) of 39.8 mA/cm^2 at an optimal thickness of 600 nm. The suggested approach might pave the way for future lead-free double perovskite solar cell design improvements and performance enhancement.

Keywords: DFT, SCAPS-1D, Cs_2SnI_6, Lead-free perovskite and optical properties

Conjugated Polyelectrolyte-Passivated Stable Perovskite Solar Cells for Efficiency Beyond 20%

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Abstract: Developing large-scale perovskite solar cells requires high-quality defect-free perovskite films with improved surface coverage. One of the most convenient ways to achieve this is through the incorporation of appropriate passivation molecules in the perovskite films. Herein, the effect of a novel conjugated polyelectrolyte, PHIA, is investigated for perovskite passivation by the comprehensive analysis of perovskite films and devices. The PHIA polymer significantly diminishes the trap states in perovskite films, and the passivated device permits lesser recombination, very low accumulation of charges at the interface, and lowers the traps which facilitated superior charge transport. As a result, a high-power conversion efficiency of 20.17% has been achieved for the PHIA-modified device. Additionally, this passivation approach effectively enhanced the long-term device stability by improving the hydrophobicity of the perovskite layer. Furthermore, a large-area device (2 cm2) has also been fabricated to demonstrate the expediency of this approach for future commercialization.

Theoretical Studies on Cs_2TeX_6 (X=Cl, Br, I): Promising lead-free vacancy-ordered double perovskite (VODP) for energy applications

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Abstract: Recently, there has been significant progress on metal halide perovskite solar cells for energy applications. Report shows that single-junction perovskite solar cells (PSCs) can reach an efficiency of around 25.7%.(1) Although the Shockley–Queisser limit indicates material having a band gap around 1.4 eV can have the optimum single junction solar cell efficiency, a few wide band gap materials can also be used for the top cell absorber layers in multi-junction tandem PSCs. Also, VODPs have recently gained attention for their enhanced stability and lead-free systems.(2) Here, we have investigated the electronic and other physical properties of the Cs_2TeX_6 VODP systems with Cl(VI), Br(VI), and I(VI) as X-anions using density functional theory (DFT) approach with PBE-GGA and mBJ approximations as implemented within the full-potential linearized augmented plane wave plus local orbital method. The band structures computed (with spin-orbit coupling) for Cs_2TeCl_6, Cs_2TeBr_6, and Cs_2TeI_6 indicate their semiconducting nature with band gap values ~ 3.11, 2.45, and 1.64 eV, respectively. Halogens' p- and tellurium's s-orbitals contribute significantly to the valance band maximum, whereas tellurium's p- orbitals play a prominent role near the conduction band minimum. Our study also suggests that Cs_2TeX_6 can be a suitable candidate for the exploration of photovoltaic and optoelectronic applications.

Keywords: DFT, vacancy-ordered double perovskite, optoelectronics, Cs_2TeX_6

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Halide Perovskite Nanocrystals and Lanthanide Complex-based Security Ink: Preparation, Stability and Anti-counterfeiting Application

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Abstract

Producing an unauthorized replica of a high-end brand is known as counterfeiting. Nowadays, counterfeiting can be found in every aspect of life, including currency, important documents, cosmetic brands, medical equipment, medicines, and food products. It is the need of the hour to develop technologies for high-security encryption to encounter counterfeiting. In this work, we have synthesized $CsPbBr_3$ nanocrystals using the hot injection method and $Eu(TTA)_3Phen$ by the chemical route and prepared bi-luminescent security ink using these luminophores (Materials Research Bulletin, 155 (2022) 111977). Lanthanide complexes and halide perovskite nanocrystals show high photoluminescence quantum yield. The luminescence security ink comprising $Eu(TTA)_3Phen$ and $CsPbBr_3$ nanocrystals offer multilevel anti-counterfeiting strategies. This ink shows a red color under UV light (367nm) and green color under blue light (450nm) excitations and hence can be used for static multi-stimuli anticounterfeiting ink. Additionally, the $CsPbBr_3$ nanocrystals show a lifetime of the order of nanoseconds and $Eu(TTA)_3Phen$ of the order of microseconds therefore, this bi-luminescent security ink can also be used for dynamic anticounterfeiting security ink. Further, we studied its photostability, chemical stability, and stability under an ambient atmosphere which will be discussed in the presentation.

Keywords: Halide perovskites; bi-luminescent security ink; photoluminescence; anti-counterfeiting; lanthanide.

Machine Learning for Bandgap Prediction of stable and efficient Perovskite Solar Cell

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Abstract: The fabrication processes of highly efficient Perovskite Solar Cell (PSCs) with/ without different interfacial layers are time consuming, costly and it required inert atmosphere. In this aspect, we have used autonomous experimentation toolkits like linear or multiple regression or various machine learning algorithms by preparing a dataset containing 155 data points, collected from recently published literatures covering various constituent properties of organic and inorganic perovskites, hybrid organic-inorganic perovskites and double halide perovskites. In this research,the dataset is analysed using Linear Regression (LR), K Nearest Neighbour, Random Forest and Neural Network algorithms for predicting the suitable bandgap of the perovskite absorber of specific composition for higher range of solar absorption. The best fited LR model has been chosen for predicting bandgap range of 1.55-3.02 eV for the perovskite absorber $Cs_aFA_bMA_{(1-a-b)}Pb(Cl_xBr_yI_{(1-x-y)})_3$ which considers the compositional engineering of cations and halide anions. The LR model shows highest R^2-value of 0.99 and that indicates best accuracy of 99% for the prepared dataset with a least Root Mean square Error (*RMSE)* 0.0617.

Keywords: Bandgap Optimization, Perovskite Solar Cell, Compositional Engineering, Linear Regression.

Perovskite Solar Cells: A Study by High-Efficiency

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ABSTRACT

Faced with the world's growing energy and environmental crises, the development of renewable energy has piqued the interest of all governments. Solar one of the most promising renewable energy sources since it is abundant and inexpensive. While solar cells are high performance have advanced significantly in recent decades, the high module cost has hampered widespread adoption of photovoltaic systems. This urgent demand for cost-effective solar cells has tremendously helped solar cell research in the last ten years. This paper examines the recent progress of low-cost, high-efficiency solar cell technology. According to this research work, perovskite solar cells are low-cost and high-efficiency. Perovskite solar cell technologies are also discussed, including their development and current state-of-the-art findings.

Keywords: Perovskite, Solar Cells, High-Efficiency, Stability

Stability Analysis Of Efficient Perovskite Solar Cell Using Machine Learning Tools

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Abstract: Over the past two decades, stability has been one of the main facets that creates a delay in the commercialization of efficient perovskite solar cells (PSCs). In this work, the degradation mechanisms for perovskite materials has been investigated and found stable perovskite material for the fabrication of PSCs. A dataset has been prepared from 140 published papers on n-i-p based organo-inorganic lead mixed halide-based PSCs and analyzed using machine learning (ML) model. The effect of various factors like Band gap, Grain size , Radius of cations and anions, Compositional ion coefficient, Goldschmidt tolerance factor(τ), Relative humidity(RH), etc., on the structural stability and efficiency of PSCs have been explored. A predictive model is flourished for stability and power conversion efficiency (PCE) using Regressions, Neural network (NN) tools for general composition of $Cs_aFA_bMA_{(1-a-b)}PbI_xBr_{(1-x)}$. The association rule mining (ARM) is used to discover the chief descriptors leading to the most stable PSCs under ambient and specific storage conditions. A groups of datasets are prepared using the chief descriptors with other features and analyze the effect on stability of PSCs. The best model named GradientBoostingRegressor gives the best accuracy with a R square value of 0.875 with RMSE value of 0.06. With this model, stability analysis and prediction is being studied.

Keywords: Perovskite solar cell(PSCs), Machine learning (ML), Stability analysis , Structural stability , Compositional study.

Effect of Antisolvents on the Optical properties of Room temperature synthesized $CsPbBr_3$ Quantum Dots

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Abstract: In recent years, all inorganic cesium lead halide perovskites quantum dots (QDs) have shown promising potentials in various optoelectronic applications such as light emitting diodes, solar cells and photodetectors. Among them, $CsPbBr_3$ QDs have shown excellent stability against oxygen, moisture, heat and light. The traditional hot injection method for QDs synthesis needs inert gas protection, high temperature, and localized injection operation that hinders its large-scale preparation. In this work, we have synthesized $CsPbBr_3$ QDs at room temperature in ambient air condition by modified ligand assisted reprecipitation method. We have selected different antisolvents, namely, acetonitrile, acetone, IPA, ethyl acetate and methyl acetate for the purification of QDs. A significant effect on optical properties of $CsPbBr_3$ QDs was found after centrifugation process. QDs purified with acetonitrile, ethyl acetate and methyl acetate have shown a slight blue shift, while IPA and acetone purified QDs have slightly red shifted compared to the QD treated without antisolvent both in UV-Vis and photoluminescence spectra. XRD pattern of the as synthesized QDs exhibit a cubic structure. This work provides a route for large-scale synthesis of $CsPbBr_3$ perovskite QDs at room temperature under ambient conditions.

Keywords: Perovskite, Quantum Dot

Bipyridine Mediated Surface Engineering of Mn-doped $CsPbCl_3$ Perovskite Nanocrystals

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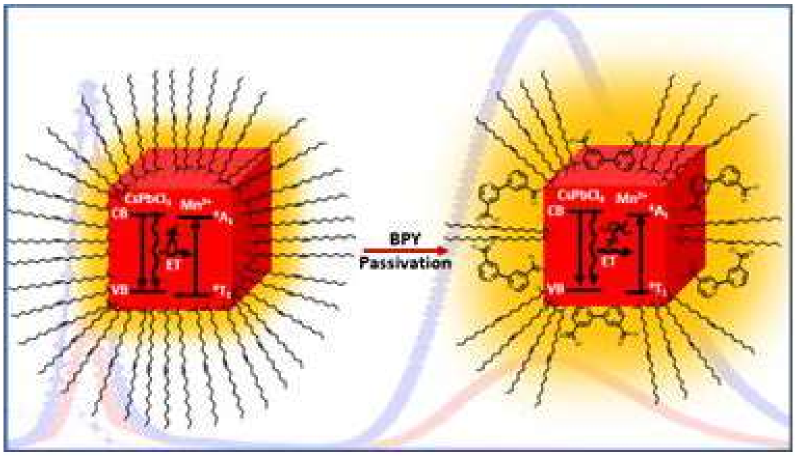
Abstract: Metal doping strategy reduces the defect/trap states and improves the stability of $CsPbCl_3$, which is beneficial for optoelectronic applications. Mn-doping in $CsPbCl_3$ perovskites nanocrystals (PNCs) has shown an improved photoluminescence quantum yield (PLQY) and stability; however, their emission is limited to trap-mediated energy transfer. Herein, we have demonstrated for the first time in improving the energy transfer properties, relative PLQY, and stability of Mn-doped $CsPbCl_3$ PNCs by the post-synthesis surface passivation with small organic molecule, 2,2'-bipyridine-4,4'-dicarboxylic acid (BPY). Here, BPY is used as an efficient passivating additive, which reduces surface defects in Mn-doped $CsPbCl_3$ via carboxyl groups and pyridine nitrogen with less coordinated Pb atoms hence, improvement of energy transfers from $CsPbCl_3$ to Mn^{2+} dopants and the relative PLQY. The relative PLQY of Mn-doped $CsPbCl_3$ PNCs has increased from 16% to 70% after post-synthesis BPY treatment. Mn-doped $CsPbCl_3$ PNCs were characterized before and after BPY passivation using various characterization techniques. The photo- and thermal stability studies under ambient conditions and UV light irradiation showed the BPY passivated Mn-doped $CsPbCl_3$ PNCs are more stable than the unpassivated one.



Keywords: Halide perovskites, Doping, Surface passivation, Energy transfer, PLQY

Nucleophile-Controlled Halide Release from the Substitution Reaction of Haloketone for Facet Tuning and Manganese Doping in $CsPbCl_3$ Nanocrystals

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Abstract Halide content of the reaction medium not only enhances the brightness of $CsPbCl_3$ nanocrystals but also, control the shape modulations as well as doping Mn(II) in these host nanocrystals. Correlating both the shape and doping, herein, an in-situ reaction of nucleophile-controlled halide release was explored for monitoring facets modulations and doping in $CsPbCl_3$ nanocrystals. This was performed using alkyl amine as nucleophile which reacted with α-halo ketone, phenacyl chloride, to release Cl^-. Increase in amine concentration released more Cl^-, reduced the possibility of shape transformation from perfect to truncated cubes during annealing. Similarly, for Mn(II) doping, the dopant photoluminescence intensity remained directly proportional to the amount of amine nucleophiles. Quality of both doped and undoped nanocrystals obtained in this procedure remained unparallel and the method provided a strong correlation of rate of halide release with both facet modulations and doping in these nanocrystals.

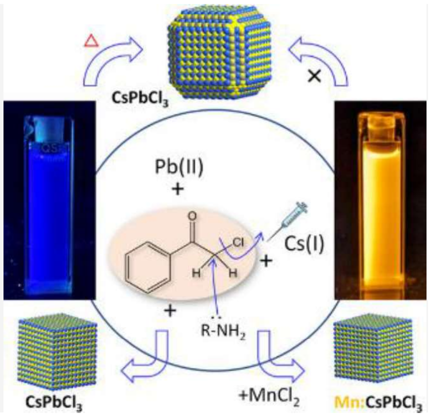

Fig.1. Schematic presentation of halide release controlled facet modulation and doping in $CsPbCl_3$ nanocrystals.

Keywords: Lead Halide Perovskite, α-halo ketone, Substitution Reactions, Annealing, Doping.

Evidence for the Field-Induced Spin-Flip Transitions in Ce substituted $GdCrO_3$

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Abstract

Heavy rare-earth perovskites especially the chromites ($RCrO_3$) with R = Pr, Ce, Gd, Sm etc. exhibit complex magnetic ordering which holds robust spin dynamics and strong exchange interactions (R^{3+}-Cr^{3+}, R^{3+}-R^{3+}, Cr^{3+}-Cr^{3+}). These systems also exhibit some fascinating physical phenomena such as spin-flip transitions, negative magnetization and compensation, multiferroic behavior and field-induced magnetic-phase transitions which play a vital role in designing spin-valve devices [1-4]. The present work deals with the structural and magnetization studies on a polycrystalline perovskite $Gd_{0.9}Ce_{0.1}CrO_3$ prepared from the standard solid state reaction technique. PPMS based temperature and field (100 Oe $\leq H_{\mathrm{DC}} \leq$ 1 kOe) dependent magnetization measurents under Field Cooled Cooling (FCC) protocol reveals the temperature and field-contolled spin-flip transition and negative magnetization phenomena which are the key features of the present investigated system. Under H_{DC}, the Cr^{3+} sublattice creates a local field to which the R^{3+} sublattice aligns anti-parallel and compensates the magnetization of the Cr^{3+} sublattice which inturn gives to negative magnetization (M_{N} ~ -7.15 emu/g at T = 3 K). The overall magnetization M(T) undergoes a second transition at the low temperatures associated with spin-flip transition triggered by the critical field, H_{C} = 200 Oe at T_{SF} (10 K). Gradual increase in the overall magnetization and cross-over due to spin-flip transition can be understood by the Zeeman interaction term $E_{zeeman} = -\mu_0 M_{\mathrm{Net}} H_{\mathrm{Ext}} \mathrm{Cos}\,\theta$, where θ is the angle between the M_{Net} and H_{Ext} [3]. In the present system the magnetic ordering prefers the Γ_4 structure in which the spins flip from $(00\bar{1})$ to (001) where, the c-axis is the easy axis. Such multiple thermo-magnetic switching of the investigated system play a significant role in the development of the field of MRAM devices.

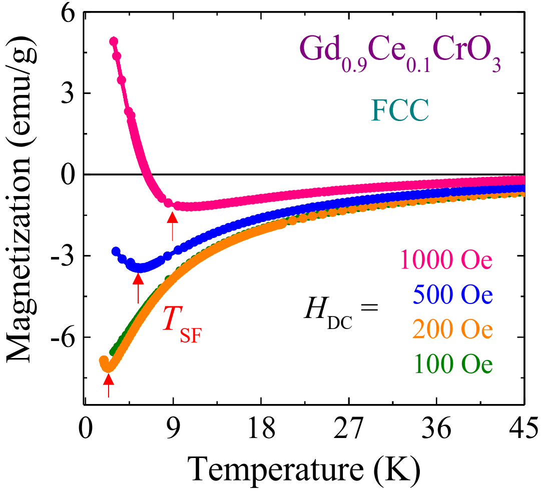

Figure. Temperature dependant magnetization of $Gd_{0.9}Ce_{0.1}CrO_3$ under the FCC protocol in the presence of different external magnetic fields.

Keywords: Gamma spin structures, Spin-flip transition, Zeeman Energy, Negative magnetization.

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A way towards lead and halide free photovoltaics

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Abstract: The height of the toxicity and instability in the Lead and Halide based perovskite photovoltaic materials have made researchers step towards Lead and Halide free perovskite materials. Chalcogenide perovskite materials are a novel class of lead and halogen-free ionic semiconductors. The optical band gap of these materials can be systematically tuned by cation and anion alloying. These chalcogenide perovskite materials are predicted to demonstrate around 30% of maximum theoretical photovoltaic power conversion efficiency (PCE); similar to the well-studied traditional lead-halide perovskites - $CH_3NH_3PbI_3$. In our lab, we synthesized the $BaZrS_3$ (BZS) and coated the films by pulsed laser deposition method. The studies of structural and optical properties of sulfide perovskite thin films revealed their potentiality towards the photovoltaic application; mainly, $BaZrS_3$, and we found that this sulfide perovskite material can be a promising absorber for solar cell application.

Keywords: toxicity; Chalcogenide; $BaZrS_3$; sulfide perovskite; absorber

Correlation between the Crystal Structure and the Intermediate Spin-states of Pr substituted $LaCoO_3$ Nanostructures

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Abstract

Electronic structure of Lanthanum Cobaltate ($LaCoO_3$) based perovskites have been the subject of intense research activity in recent years because of their unique spin state equilibria and magnetic behavior. The *d* electrons of trivalent cobalt ions at the center of oxygen octahedral cage in the perovskite lattice are very susceptible to the crystal field splitting. Subtle balance between the such crystal field energy and Hund's coupling of Co^{3+} ions controls the spin-state of electrons present in the *d* orbitals [1,2]. The current research work is focused on such diverse intermixed spin states of electrons in Co^{3+} ions of $La_{1-x}Pr_xCoO_3$ (LPCO) perovskites which have strong correlation with the crystal structure and magnetic properties. Nanostructures of LPCO for various compositions ($0 \leq x \leq 0.9$) have been synthesized by means of the sol-gel technique involving moderate heat-treatment (600^0C) which leads Nano size particles of size 32-37 nm for dilute compositions of Pr. The crystal structure analysis performed by the *X*-ray diffraction and Rietveld Refinement reveals a well-defined phase transition from rhombohedral phase (*R-3c*) to orthorhombic (*Pbnm*) upon increasing the composition from $x = 0$ to $x = 0.6$ which exhibit ferromagnetic behaviour (Fig. 1). However, the bulk grain size samples exhibit monoclinic (I2/a) to orthorhombic (*Pnma*) phase transition due to the dominant Jahn-Teller (J-T) distortion (Fig.1). The J-T distortion factor is controlled by the intermediate spin state of Co^{3+} spins of $t_{2g}^5\ e_g^1$ configuration. The magnetic and structural analysis reveals that the intermediate spin-state of Co^{3+} electron is more prominent in bulk $LaCoO_3$ than the nanostructures of $LaCoO_3$ (Fig.1). The Pr substitution at A-site induces a shorter Co−O bond length owing to the smaller ionic radius of $Pr^{3+/4+}$ as compared to La^{3+} ions. A systematic study on the role of J-T distortion and its influence on the structural and magnetic properties of the LPCO system will be presented.

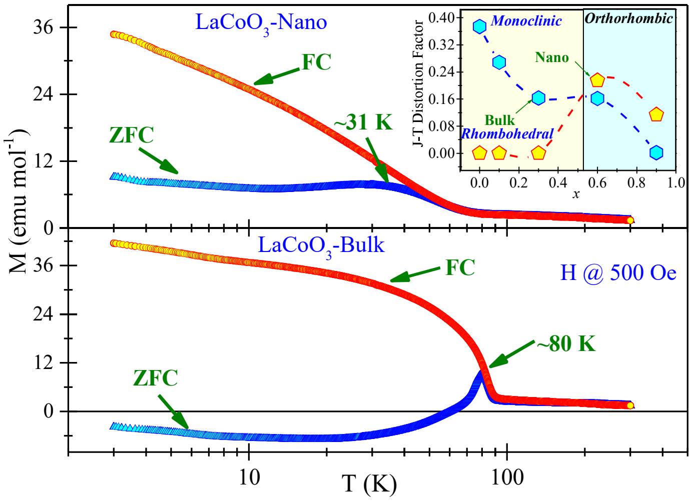

Fig. 1: Temperature dependence of the magnetization recorded under zero-field-cooled (ZFC) and field-cooled (FC) conditions in an external field H = 500 Oe for (a) $LaCoO_3$-Bulk (b) $LaCoO_3$-Nano. Inset shows the composition variation of J-T distortion factor for $La_{1-x}Pr_xCoO_3$ bulk and nanostructures.

Keywords: Perovskites, Jahn-Teller Distortion, Intermediate spin state

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Charge Carrier Dynamics in Curcumin Based Dye-Sensitized Solar cells

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Abstract: In recently, dye-sensitized solar cells (DSSC) have become a good competitive alternative to the traditionally used silicon-based solar cells, due to their low-priced and ease of fabrication. Dye, used as a photosensitizer, is one of the utmost components of DSSCs. However, many types of sensitizers have been employed into the DSSCs. Among these, natural sensitizers have been shown to be more cheap, more availability, nontoxic and environmentally friendly photosensitizers. This paper reveals the charge carrier dynamics of curcumin based DSSCs using impedance and modulus spectroscopy in dark and with subsequent light-on and -off conditions. Nyquist plot that confirms the non-Debye type relaxation in this curcumin DSSC under both dark and illumination conditions. We found that the power conversion efficiency of curcumin based DSSC is 0.4%. The results show the enhanced performance of the DSSCs in terms of charge transfer, transport processes and power conversion efficiency.

Keywords: Natural dyes, sensitized solar cell, Impedance, charge carrier dynamics,

Enhanced Photoelectrocatalytic Activity Towards the Reduction of CO_2 to Alcohols on $Cu_{(2-x)}O(x=0,1)/SrTiO_3$ Photocathode Heterojunction

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Abstract: Photo electro catalytic reduction (PECR) of CO_2 to value added chemicals and fuels will reduce the dependency of fossil fuels, and at the same time it will solve the environmental issues such as unevenness in the temperature, rains and rise in sea levels [1]. In order to reduce the CO_2, a heterojunction of Cu_2O was electrodeposited on FTO glass substrate [2] and on top of it a solution processed spin coating of $SrTiO_3$ was deposited and annealed at different temperature range of 300-600 °C. The crystalline phase formation was confirmed by XRD, and the optical behaviour of the synthesised heterojunction was carried by DRS-UV-Visible Spectrum. Electroanalysis of the synthesised heterojunctions were done by Linear Sweep Voltammetry (LSV), Electrochemical Impedance Spectrometry EIS) and Chronoamperometry (CA) for charge transfer behaviour and Photo electrocatalytic activity toward the CO_2 reduction. Liquid products of Methanol and Ethanol were identified and quantified by using Gas Chromatography at different period during the reactions as well as at different applied potential. Enhancement in the formation of Methanol and Ethanol was identified on heterojunction as compared to the pristine Photo electrocatalyst.

Keywords:

Photoelectrocatalytic reduction (PECR), $Cu_{2-x}(x=0,1)O/SrTiO_3$ heterojunction, Electrodeposition, Spin coating, CO_2 Reduction

References:

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Ultrafast Charge Carrier Dynamics of Cs_2SnI_6: A promising Lead Free Perovskite

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Cs_2SnI_6 has lately entered the race for being a prospective lead free photovoltaic absorber thanks to the remarkable solar efficiency numbers displayed by it. However the full potential of this material still lags far behind than that otherwise anticipated. Insufficient research of its photophysics can be one major reason to blame. So here in this work we have curtailed this gap in knowledge. To begin with, theoretical calculations were carried out to determine the whereabouts of the excitons in the Brillouin zone of Cs_2SnI_6. Following these assignments, we employed TA spectroscopy to look at their temporal development. Here we discovered that the decay of high energy excitons was significantly delayed. Even more intriguing, these high energy excitons still appeared even when the energy of the incoming photons was inadequate. Furthermore, transient mobility measurements showed that hot carriers (HCs) have higher mobility than cold carriers, contrary to what is commonly encountered. This implies that HCs in Cs_2SnI_6 experience fewer carrier-phonon scattering events. In conclusion, our results propose that Cs_2SnI_6 may be a good choice for HC - based solar cells since it encounters fewer HC scatterings and exhibits delayed decay of its high energy excitons, which are two prerequisites for such devices.

Surface passivation to improve carrier mobility and life-time in double cation perovskite material for inverted perovskite solar cells

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Abstract: Formamidinium (FA) based halide perovskite material has got tremendous research interest as a replacement of MA counterpart in the 3D perovskite structure in order to improve the thermal stability. However, the serious phase instability issues and low defect formation energy of FA-based perovskite compromise the solar cells' long-term stability and efficiency. In order to increase the stability of the photo-active -phase of the perovskite structure, we have optimised the FA-based perovskite structure $Cs_{0.1}FA_{0.9}PbI_3$ by adding a small proportion of Cs cation to the perovskite structure. The surface defect that seves as non-radiative recombination centre originated during the crystallization of the perovskite phase reduces the mobility and life-time of the photo-generated charge carriers and hence Voc and FF during their collection. In order to improve the device efficiency and hence stability we have incorporated 3,5-bis(trifluoromethyl)phenyl isocyanate small additive molecule that strongly combined with the uncoordinated ions in the perovskite structure With the improvement of all photovoltaic parameters, the modified device exhibits an average PCE of 17.35% as compared to the 14.33% of the pristine device.

Keyword: perovskite solar cell, defect passivation, phase stability, compositional engineering, thermal stability.

Analytical Modelling and Temperature Dependent Current Analysis of Hybrid Perovskite-based Memristive Devices

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Abstract: This work presents the use of lower-dimensional butyl amine lead iodide (BA_2PbI_4) perovskites to fabricate memristive devices using a simple solution processing technique, and their resistive switching properties are studied. The 2D perovskite memristor exhibits SET and RESET voltages of 0.64 V and -0.33 V, respectively, along with an ON/OFF ratio of $1.36x10^3$. The repeatability test of the resistive switching using fast voltage pulses yields a cyclic endurance of 1050 cycles and state retention for 1350 seconds. From the I-V characteristics in the temperature range of 200K to 300K, the current conduction mechanisms in the low resistance state and high resistance state are found to be ohmic and tunnelling-dominated, respectively. Besides, a novel strategy to mimic the memristor characteristics is presented using experimental data fitting and SPICE simulation. The model is based on the standard Yakopcic model of memristor. The fitting results of the experimental I-V plots of the fabricated perovskite devices to the model equations yield a per-cycle mean error of 2.76% and 11.67% in the SET and REST cycles, respectively. Such modelling of memristor characteristics will be helpful in incorporating memristors in circuits and system design tools.

Keywords: Perovskite Memristor, SPICE modelling, ON/OFF ratio, Endurance, Retention.

Perovskite NanoCrystals Based Light-Emitting Diodes

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Abstract: The successive breakthroughs in metal halide perovskite (MHP) based solar cells have led to their intensive exploration by the research communities as photo-emissive layers for light-emitting applications. This is owing to their excellent optoelectronic properties such as high photoluminescence quantum yields (PLQYs), widely tunable bandgap, colour-purity, and low temperature processing. In the field of perovskite light-emitting diodes (PeLEDs), external quantum efficiency (EQE) is a commonly used metric to evaluate device performance. One of the major factors that govern the EQE of PeLEDs is PLQY of perovskite emitters. Large PLQY values of perovskites are desirable for obtaining an efficient LED. Zero-dimensional colloidal perovskite nanocrystals (PNCs) are one such class of highly luminescent perovskite emitters resulting from restricted size of a bulk perovskite in multiple dimensions. The excitons in such a system are tightly quantum confined and thus increase the radiative recombination at low excitation densities required for LED operation. The use of PNCs as emissive layer in PeLEDs have led to great enhancement in EQE values and open room for further improvements employing device engineering and additive treatment approaches. I will be talking about synthesizing room-temperature based PNCs to be used for fabricating green, red and blue LEDs for display applications.

Keywords: Metal halide perovskites (MHPs), Perovskite light-emitting diodes (PeLEDs), External quantum efficiency (EQE), Photoluminescence quantum yield (PLQY), Perovskite nanocrystals (PNCs)

Temperature Driven Charge Transfer Process in Quantum Confined Two-Dimensional Mn-doped $CsPbBr_3$ Perovskite Nanoplatelets

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Abstract: Temperature dependent transient absorption study has been demonstrated for highly quantum confined Mn^{2+} doped $CsPbBr_3$ nanoplatelets, which showed the diverging behaviour in the energy/charge transfer process. Upon lowering the temperature to 5 K, energy/charge transfer process in Mn-$CsPbBr_3$ nanoplatelets has been suppressed than that of 300K, owing the trapping of charge carriers in Br vacancy state, which is near to the conduction band of $CsPbBr_3$. Consequently, at 300 K thermally active carriers efficiently de-trapped from the defect states along with strong exciton-phonon coupling leading to the efficient energy/charge transfer process. The detailed understanding of the energy/charge transfer mechanism of highly confined two-dimensional Mn-$CsPbBr_3$ nanoplatelets through temperature dependent transient study may pave to design and fabrication of highly efficient optoelectronic as well as photovoltaic devices.

Keywords: Perovskites, nanoplatelets, defect state, energy/charge transfer, ultrafast spectroscopy,

Fabrication of Perovskite Solar Cells Using Nanorod Shaped TiO_2 Electron Transport Layer

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Abstract: Organic-inorganic hybrid perovskite solar cells (PSCs) have promoted a surge of research in academics and industry in recent years because of their unique properties like long carrier diffusion length, high amount of light absorption, tuning of bandgap and other advantages like solution fabrication process, and low cost of raw materials. This work focuses on fabrication of PSC using nanorod shaped TiO_2 as electron transport layer (ETL). A simple hydrothermal method is used for the fabrication of nanorod shaped TiO_2. Scanning electron microscopic (SEM) image (shown in Fig. 1) confirms uniform shape of nanorod TiO_2 having average diameter as 200 nm. XRD pattern of TiO_2 confirmed the rutile phase and calculated crystallite size of 27.542 nm. The nanorod structured TiO_2 gives increased surface area and improved charge transport properties, making it desirable for ETLs. For the fabrication of PSCs spin coating method is used at room temperature and electrical characterization conducted at *AM 1.5G* illumination. The V_{oc}, I_{sc}, fill factor (*FF*) and cell power conversion efficiency (η) of $MAPbI_2Cl$ is calculated to be 2.9V, 1.67 mA and 1.44 mW and 2.89%. The fabrication of both ETL and PSC have been performed under ambient atmosphere without any controlled environment.

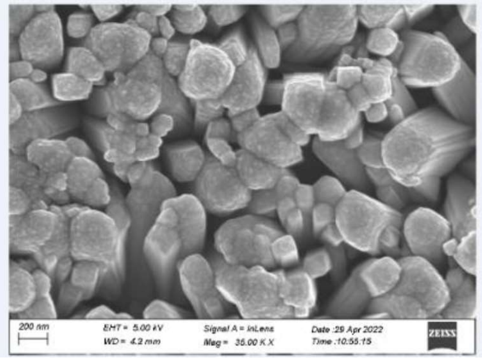

Fig.1: SEM image of fabricated nanorod shaped TiO_2 used as ETL for PSC.

Keywords: Perovskite solar cells, Nanorod shaped TiO_2, Electron transport layer, Spin Coating, Hydrothermal treatment.

Title: Copper(I) thiocyanate (CuSCN) as a hole-transport material in transparent Perovskite solar cell

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Abstract:

Copper thiocyanate(CuSCN) is highly transparent, very stable, offered as a low-cost alternative to current organic and inorganic metal oxide hole-carrying materials, and simple to the solution process. This work describes the creation of a thin film of copper(I) thiocyanate (CuSCN) as hole transport layers (HTLs) made from aqueous ammonia for the fabrication of perovskite solar cell. The deposition method involves CuSCN being directly dissolved in Ammonia and distills water and stirred at room temperature for about 3 hrs. The deposited thin film was characterized by XRD and UV-VIS spectroscopy for their structural and optical properties respectively. The diffraction peak was observed at 13.260˚ to 34.285˚ corresponding to the plans (001) to (212). The Dislocation density (δ), Crystallinity size (D) nm, and Micro strain(ε) of CuSCN are $0.0018 nm^{-2}$, 23.04nm, and 0.008. The optical bandgap of CuSCN is 3.10eV(direct bandgap) and 2.91eV(indirect bandgap) obtained from the UV-VIS characterization data. It allows transparency for visible to near infrared in the electromagnetic spectrum.

Keywords: CuSCN, Perovskite solar cell, Hole transport layer.

Electron rich inorganic Hole-Transporting material for high efficient perovskite solar cells.

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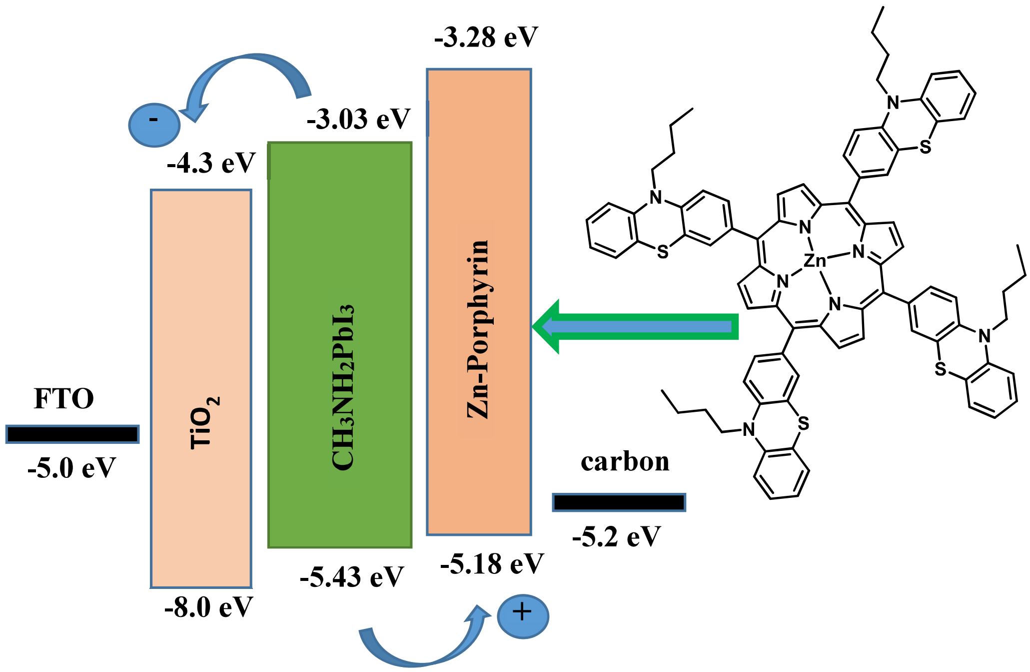
Abstracts

We know that high efficient perovskite solar cells successfully discovered a decade ago but the development of low cost and high efficient hole transporting material for perovskite solar cells has still some research gap. Here a material is synthesized having a property of electron donating and enhance hole attracting property. Zn-Porphyrin has a π conjugated system bearing phenothiazine electron donating moieties permit obtaining highly efficient hole transport material.



Synthesis And Characterization of Cr doped BZT ceramic with Perovskite like structure

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Abstract:

Perovskite-like ceramics, BZT ($BaTi_{0.90}Zr_{0.10}O_3$), and Cr-BZT ($BaTi_{0.89}Cr_{0.01}Zr_{0.10}O_3$) were prepared by solid-state reaction technique and studied ferroelectric properties by P-E hysteresis loops. These ceramics were synthesized at sintering temperatures of 1200°C, 1250°C, and 1300°C and evaluated for elemental composition for perovskite-like structure. We reported frequency-dependent ferroelectric behavior of BZT and Cr-BZT at room temperature for various frequencies of 50 Hz, 100 Hz, 150 Hz, 200 Hz, and 250 Hz. The Electric coercivity (E_c), Remanent polarization (P_r), and Saturation polarization (P_s) were investigated at different sintering temperatures at 50 Hz for both the samples BZT and Cr-BZT. The structural and surface properties of the produced ceramics were examined by using X-ray diffraction (XRD) and scanning electron microscopy (SEM). The ferroelectric properties can be related to structural characteristics. To investigate ferroelectric phase transition temperature, the temperature dependence of relative dielectric constant (ε_r) and dielectric loss tan(δ) were determined. The ferroelectric characteristics of the produced ceramics were examined as a function of Cr and Zr concentration with respect to sintering temperature. A complex impedance study "CIS" was used to have information about the conduction mechanism in the prepared perovskite-like ceramics.

Keywords: Perovskite Structure; BZT; Cr-BZT; PE Loop; Solid-state reaction

Stable Single Precursor synthesized from Low Grade PbI_2 using Sono-chemical Approach for Economical and Efficient Perovskite Solar Cells

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Abstract: Commercialization of perovskite solar cell (PSC) technology is hampered by high-cost device fabrication techniques and inadequate stability under ambient conditions. In this study, we used low-grade PbI_2 to make highly stable Methylammonium lead Iodide ($MAPbI_3$) powder via sono-chemical method, in order to reduce the cost of the PSCs. The sono-chemical method is used to synthesize $MAPbI_3$ microcrystals because of its significant advantages, including morphological control and educt dissolution support. The tetragonal phase of the synthesized perovskite ($MAPbI_3$) powder was confirmed using PXRD measurement. The synthesized $MAPbI_3$ powder was then subjected to series of analysis, including UV-Vis-NIR absorption, PL Emission, FT-IR, and TGA. The FESEM and TEM analysis reveals the size of synthesized $MAPbI_3$ microcrystals are in the range of 0.3-2 µm. The optical and photovoltaic properties of conventional solution-based films and powder-based recrystallization films were studied and compared their performance in the Carbon based Perovskite Solar Cell (C-PSC). The powder based solar cell exhibits slightly higher power conversion efficiency (10.1 %) than the device fabricated by conventional solution-based approach (9.5% for high grade PbI_2 + MAI and 6.8% for low grade PbI_2 + MAI). The enhanced photovoltaic characteristics of the recrystallization-based devices were attributed to the homogeneous perovskite film with large grain size and high crystalline properties.

Keywords: Carbon electrode; Single precursor; Micro crystals; Perovskite powder; Recrystallization.

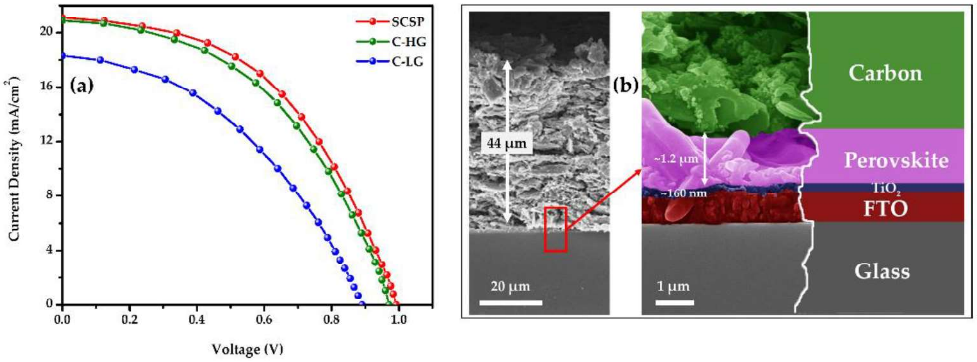

Figure 12. (a) Comparison of J-V curves of SCSP, C-HG and C-LG based C-PSCs and (b) Cross sectional FESEM images of the devices

Analysis of Read Margin and Maximum Array Size of a Hybrid Perovskite Memristor Crossbar using SPICE

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Abstract: In this work, simulation of the resistance switching characteristics of a hybrid perovskite memristor is carried out using a modified Yakopcic model in SPICE. The simulation parameters are extracted by fitting the experimental data of an in-house fabricated hybrid perovskite memristor. In practical applications, these memristors need to be implemented in the form of a crossbar array, where the sneak current is a major issue that limits the maximum implementable size of the array. The SPICE model is used for a memristor crossbar array simulation, and two different read techniques are studied: one bit-line pull-up, rest floating and all bit-line pull-up with and without gating the device. The optimum pull-up resistance is calculated analytically, and the corresponding read margin for various array sizes and ON/OFF ratios are calculated from the simulation. For our hybrid perovskite memristor, with an ON/OFF ratio of 10^3 and a read voltage of 0.1 V, a 4x4 array simulation yields a read margin of 20 mV. This margin is improved by more than 100% in the case of 1 transistor-1 memristor (1T1R) configuration for the same array size. Further, various sneak path minimization techniques have been studied to improve the read margin and, thereby, the maximum possible size of the crossbar array.

Keywords: Memristor, SPICE, Crossbar Array, Sneak Current, Read Margin.

Investigating the effect of energy level tuning by Mott-Schottky analysis on the photovoltaic performance of $FACsSnI_3$ perovskite solar cells

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Abstract

The phase stability of $FAPbI_3$ perovskite solar cells (PSCs) has been a serious concern. The black stable α-phase of $FAPbI_3$ transits into a hexagonal non-perovskite yellow phase because of a large tolerance factor (>1). Many studies reported that the incorporation of Cs^+ into the $FAPbI_3$ can tune the tolerance factor resulting in improved thermal and phase stability of the device. In this study, we have optimized device architecture $FTO/IDL1/ZnSe/FA_{0.75}Cs_{0.25}SnI_3/IDL2/CuI/Au$. This work aims to explain the charge carrier collection, transportation, and recombination mechanism at the perovskite/charge transport layer (CTL) interface. Further, the impact of band offset i.e. conduction band offset (CBO) and valence band offset (VBO), the thickness of the active layer, and operating temperature on the photovoltaic parameters have been studied. Additionally, the physics behind the formation of cliff and spike structures at the interfaces has also been discussed in detail. Simulation results revealed that the spike structure at CBO of (+0.2 eV) and at VBO of (+0.3 eV) developed at the ETL/perovskite interface and perovskite/HTL interface respectively will aid the device performance. However, large spikes and cliffs could degrade the cell performance. After using all the optimized parameters, the device achieves an efficiency of 23.08%.

Keywords: Lead-free perovskites; energy band offset; spike and cliff formation; thickness optimization; operating temperature.

Seeded Ultrathin Silver Film as a Transparent Electrode for Opto-Electronic Applications

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Abstract

Ultrathin, ultrasmooth silver(Ag) films have been the noble-metal choice in optoelectronics for widely used applications such as transparent electrodes, photovoltaics, plasmonic devices, organic LEDs, touchscreens panels, and many more. It is known that Ag thin films deposited by physical vapor deposition technique leading to island-like growth rather than continuous network typically exhibit high electrical resistivity and rough surface morphology with larger grain size. However, higher percolation thickness leads to inherent reflection losses when the Ag film is used for transparent electrode applications. Here in this work, we have shown an effective way to achieve a highly percolated, transparent ultra-thin film (<10 nm) of Ag with the incorporation of a thermally oxidized sub-nanometric copper (Cu) layer. We have reported that the use of a thermally oxidized Cu seed layer causes very low RMS surface roughness (<1 nm) of Ag films with electrically conductive Ag films with thickness as low as 2nm were realized. In addition, with the use of wide band-gap semiconductor seed layer, the Ag film showed higher transmittance especially in the longer wavelength regime. The Ag film with the addition of oxidized Cu films presents itself as a better alternative to pure Ag and other semi-transparent conducting films.

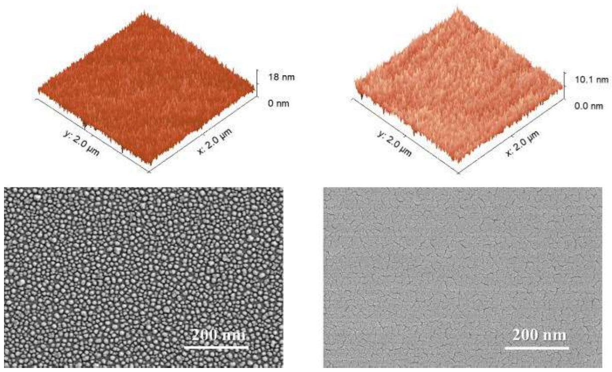

Figure 1. Three-dimensional AFM and SEM images of Ag(3nm) (left) and Cu_Oxd/Ag(3 nm) (right) substrate

Keywords: Silver, transparent electrode, ultrathin film, seed layer, percolated

Photonically Cured Solution Processed SnO_2 Thin Films for Perovskite Solar Cells and mini-Modules

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Abstract: High-throughput manufacturing of the metal-oxide thin films is limited by high temperature thermal processes with hours of processing time. This leads the thin film fabrication to impractically long annealing tools at high web speeds in Roll-to-roll fabrication of solution-processed perovskite solar cells (PSC), eventually making this technology non-viable for commercial applications. Here, an ultrafast process to anneal tin oxide thin film is investigated which is employed in PSC fabrication.

Photonic curing process is used for the rapid annealing of tin oxide layer (both compact and colloidal layer) with fine-tuned high energy pulses with milliseconds exposure time to the substrates. Temperature of the thin film is controlled by well-defined setting of operating voltage, pulse frequency and pulse width of pulses. The parametric optimization is done with the help of analyzing the chemical properties of the material formed and the same parameters are used in the device fabrication as well with power conversion efficiency of 21.1%.

Without any conventional encapsulations, the devices maintained 80% of the initial performance after 3 months in intermittent measurements and 70% stability after 150 hours with maximum power point tracking. Furthermore, the process is scaled up to 16 cm^2 area to fabricate series-connected mini-modules with 18.2% efficiency.

Keywords: Photonic curing, high throughput, SnO_2, mini-module.

Influence of Material Property of Layered Perovskite Photodetector using Machine Learning

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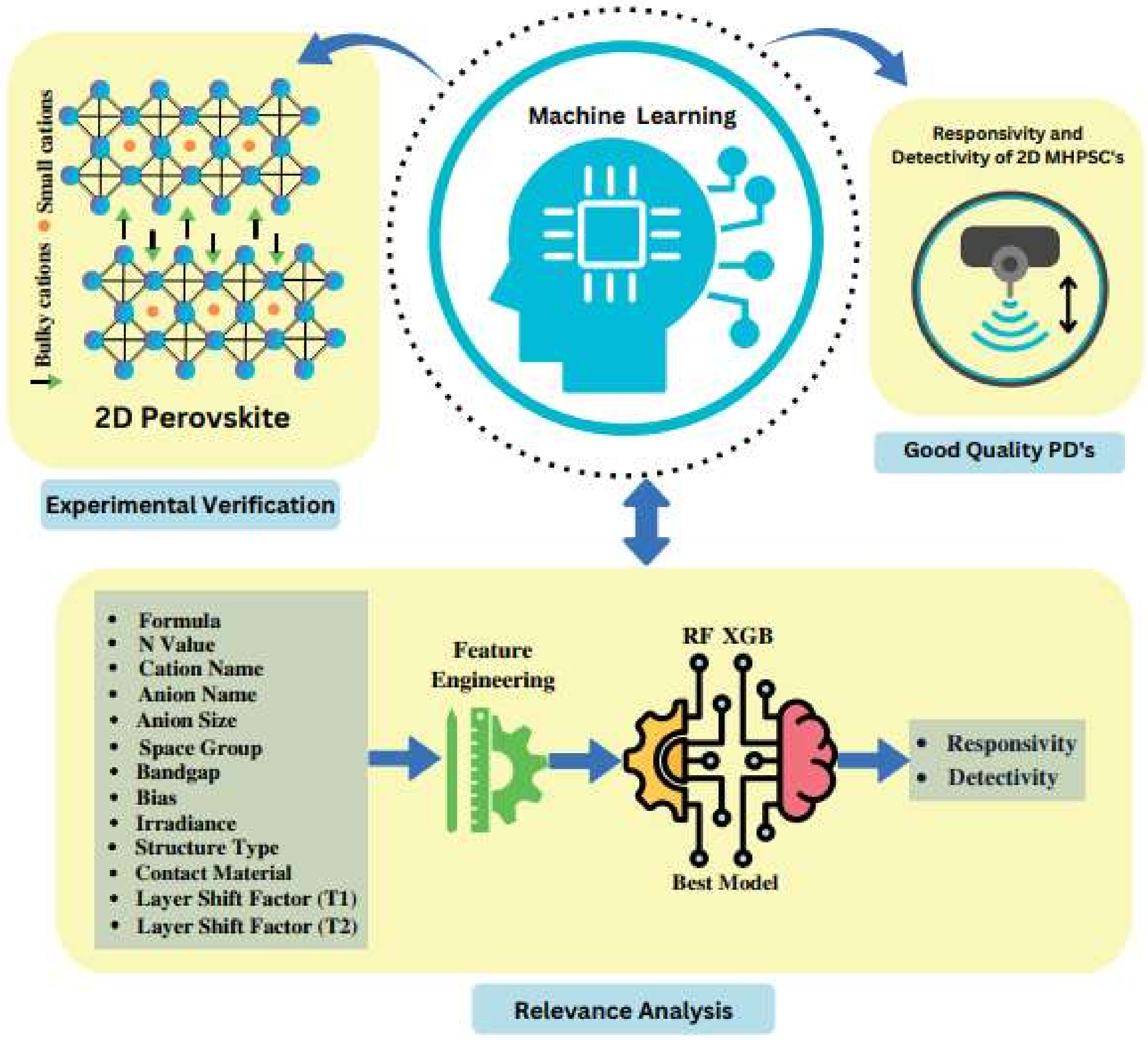
Abstract:

Two dimensional (2D) Metal halide Perovskite Photodetectors (MHP-PDs) have attracted significant attention owing to their promising performance with high responsivity and detectivity compared to the 3D congeners. In view of this, in this article we have prepared dataset by reviewing more than 100 papers reported for high quality 2D MHP-PDs to predict responsivity and detectivity using machine learning (ML). Additionally, to reason out the material properties governing the responsivity and detectivity, the descriptors chosen are layer thickness of inorganic octahedral (n), layer shift factor (t1), cation name, anion name, anion size, space group, bandgap, contact material and structure type for various compositions along with the experimental conditions as other descriptors. The predicted values are very close to the actual values for test data showing good accuracy for the developed model. Further validation of model is performed on data from literature as well as experimental data with five different 2D MHPSC PDs. The residual error between the predicted value and actual value are found to be very less. It was found that bandgap and contact material are most influencing properties in predicting the responsivity and detectivity of 2D MHPSC PDs. Thus, this study gives insights into the use of

ML techniques in improving device performance and accelerating material and device optimization.

Keywords: Machine Learning, Halide Perovskites, Single crystals, Photodetectors



Porphyrin as efficient Hole Transporting materials for Perovskite Solar Cells

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Abstract: Solar photovoltaics draws its genesis from plant photosystem.Nature provides the easiest way to capture radiant energy of sun even in low light intensity. The magnesium center of chlorophyll is an essential light harvesting unit in plants. For the technical imitation of photosynthesis, however, copper or zinc are used as central atoms, since isolated chlorophyll easily disintegrates.In this regard the macrocyclic ring chlorin which is a reduced porphyrin at one pyrrolic ring plays a crucial role in mimicking photosynthesis. Porphyrinoids has contributed their fair share in solar cells as sensitizer in dye sensitized solar cells (DSSCs) and in oganic solar cells (OSCs).With the advent of perovskite materials which demonstrates much high absorption property, ambipolar charge transport and outstanding durability and excellent flexibility, perovskite solar cells (PSCs) have gained power efficieny comparable to silicon based commercial solar cells.However poor heat and moisture stability hinders it's commercialization.

In order to provide stability and replace the traditional hole transporting layer we have designed some triphenylamine and pyrene based donor appended porphyrin materials which can be used as HTMs. The thermal analysis shows high stability opto 300°C. The HOMO-LUMO band gap is comparable with perovskite material to enhance charge-transport properties, thus making feasible a sequential improvement of the efficiencies of the PSCs. As the fabrication of devices based on these materials still require high-temperature sintering process or vacuum-process,our porphyrinoids are thermally stable.HTMs play an important role in improving the performance, which can facilitate hole extraction and transfer, suppress charge recombination and enhance stability. Porphyrin analogues not only serves as cheaper and efficient materials for HTMs in perovskite device but also improves device stability against environmental degradation and also for encapsulating the device for long term stability.

Keywords: Porphyrinois, Hole transporting materials, environmental stability, encapsulation,

Efficient hole extraction

Insight into the mobilized and immobilized state single molecule blinking dynamics of FAPbBr3 perovskite NCs

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An inclusive understanding of excited charge carrier dynamics is imperative for furthering optoelectronic applications of semiconductor nanocrystals. Our recent study on Formamidinium Lead Bromide (FAPbBr3) NCs provide a comprehensive description of their blinking dynamics synthesized by hot injection method. The studies show the defect tolerance of FAPbBr3 NCs are really superior than that of chalcogenide QDs which is evident from their sharp PL band and greater on state residence time. In this work we have been studied 30 NCs with two different wavelengths as well as two different powers. The power dependency of the fall off time was analyzed carefully by using more number of excitation intensities. The on state probability distribution gives the values of m < 1.25 and the value of τ_c >0.7s showing that they consist of a longer on durations than chalcogenide Quantum dots. Essentially this sudy shows immobilised single particle pictures of FAPbBr3 NCs, but the immobilised state blinking dynamics suffers from surface interaction as well as milli second binning time values restricts the probing of faster processes. Keeping this in mind, we have also investigated the freely diffusing state blinking dynamics using Fluorescence Correlation Spectroscopy (FCS). The dynamics from the two different perspective investigates how the average on-off time as well as the trap state heterogeneity can vary in different environment.

Keywords: *perovskites, FAPbBr3, blinking, FCS*

Long Range Binding of Defect Clusters Leading to Suppressed Ion Mobility in Cs-Doped Methylammonium Lead Iodide

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Compositional mapping in halide perovskites by replacing A cation (in ABX_3) cation like Cesium improves the inherent stability of the perovskite structure[1,2]. In the current work, force field based atomistic simulations are performed in GULP to understand the effect of Cs concentration on ionic migration in Methylammonium Lead Iodide. Nudged Elastic Band simulations were used to calculate the Iodine ion activation barrier varying the size of supercell to obtain different Cs concentrations. Iodine migration in $CH_3NH_3PBI_3$ is conventional vacancy hopping through immediate neighbouring positions[3] as depicted in figure 2a. We have found that there are typically two classes of jumps taking place within the polyhedral frame with different migration barriers as shown in figure 1. Class I jumps participate dominantly in the macroscopic diffusion due to their low migration barrier. The activation energy barrier of Iodine jumps which occur within the octahedral is found to increase in the doped Cs-MAPI when compared with the un-doped one at different concentrations of Cs(x = 6.25%, 8.33%, 12.50%), thus ion migration is suppressed leading towards a more stable structure of perovskite.

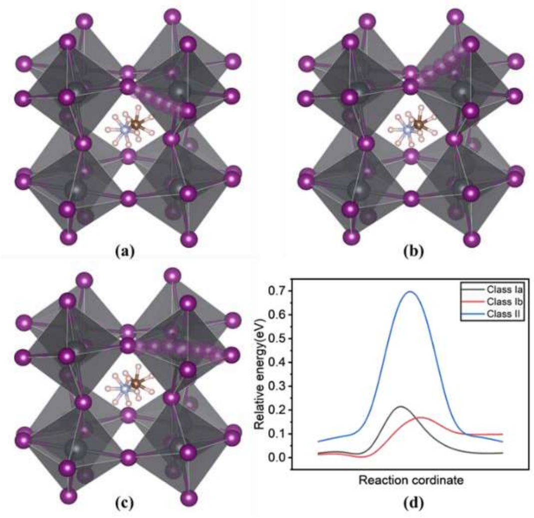
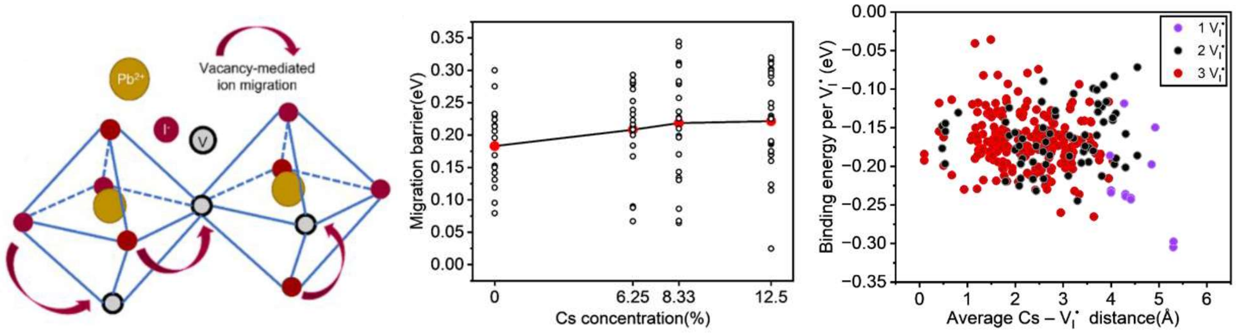

(a) (b) (c) (d)

Figure 1. Iodine ion migration paths for (a) classI horizontal, (b) class I vertical, and (c) class II jumps, (d) Migration barriers for the three classes oj jumps

Binding energy per vacancy was calculated for the $Cs - V_I$ defect clusters containing 1,2, and 3 Iodine vacancies as seen in figure 2c. It is seen that the binding energy is a long-range effect, since a single vacancy cluster are energetically favourable till 10 Å radius with a binding energy of 0.2 eV. The long-range defect binding reduce the number of mobile defecrs in the system since an extra amount of energy is required in the form of binding energy to detach V_I from Cs. Long range effect of Cs is also responsible for the relatively less significant role of Cs concentration on the migration barriers as in figure 2b, as a low concentration of Cs will also be able to do the same job as higher concentration due to long range nature of interaction.



(a) **(b)** **(c)**

Figure 2. **(a)** Schematic picture of vacancy mediated ion migration process in perovskite. **(b)** Scatter plot of Iodine migration barriers as function of Cs concentration for class I jumps. Multiple point for a single concentration correspond to different ionic jumps and red filled circles correspond to the average value of migration barrier. **(c)** Binding energy per iodine vacancy for defect clusters of one Cs_{MA} and one to three V_I. Negative values indicate energetically favourable binding.

Keywords: Ion migration , Nudged Elastic Band , Activation barrier , Binding energy

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Probing of Excitonic Transitions in All-inorganic Perovskite Quantum Dots ($CsPbX_3$: X= Cl, Br, I) by Magnetic Circular Dichroism Spectroscopy

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Abstract: Higher-order electronic transitions of all inorganic lead halide perovskite nanocrystals (NCs) ($CsPbX_3$: X= Cl, Br, I) are hardly detected by traditional spectroscopic techniques due to the condensed electronic level of NCs. In this work, we introduce a high-resolution absorption spectroscopic technique - magnetic circular dichroism (MCD), to probe all the electronic transitions and their nature through sensitive Zeeman responses to the electronic states. In particular, the MCD spectrum of the first excitonic transition changes its sign upon varying temperature and composition. Analysis of the MCD data reveals the sign and magnitude of the exciton g-factor, which depends on the strength of splitting in the conduction band due to the spin-orbit coupling interaction. This work provides a simple but efficient way to probe different electronic transitions, and experimental determination of the g-factor will help in understanding the behaviour of excitons in magnetic fields, which is helpful for a wide range of applications, including spintronics, quantum computing, and optoelectronics.

***Keywords**: Excitonic transitions, Zeeman splitting, exciton g-factor, Perovskite nanocrystals, Magnetic Circular Dichroism.*

Room-temperature photoluminescence in Mn^{2+} doped Layered Double Perovskite

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We demonstrate doping the transition metal cation Mn^{2+} in two-dimensional layered double perovskites (2D)) LDP, by solution-processed crystallization method, which results in broadband emission at ambient conditions and expansion of host lattice on increasing dopant concentration. Higher dopant feed ratio in this wide band-gap material leads to the absorption at 2.95 eV due to the $^6\mathrm{A}_1(^6\mathrm{S}) \rightarrow {}^4\mathrm{A}_1(^4\mathrm{G})$ transitions on Mn^{2+} centers. First-principles calculations based on density functional theory (DFT) confirms that at higher doping, along with the substitutional sites, Mn^{2+} dopants occupy the interstitial sites too, resulting in lattice expansion. The potential of Mn^{2+} to improve optical and magnetic properties of host lattice and a deeper understanding of distribution of Mn^{2+}dopant, makes these LDPs a promising material for emitters for solid-state lighting, and magneto-optical applications.

Quasi Interdigitated Back-contact-perovskite solar cells using Nano-Imprint Lithpgraphy

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Abstract: The conventional perovskite solar cells have reached an efficiency of ~25% in recent times in which the thin perovskite film, which acts as an absorber layer is sandwiched in between the hole/electron collection layers on the top and bottom. However, such device configuration poses several inherent problems namely - the risk of pin holes in the perovskite thin film causing shorting between the electrodes, the deposition of the top contact damaging the chemically sensitive perovskite layer and not achieving 100% area for photocurrent generation. These problems can be addressed by adopting a robust back-contact solar cell architecture where both cathode and anode are positioned at only one end of the photo absorbing layer. The back-contact structure of solar cells consists of a hole selective contact like Ni/NiO_x and electron selective contact like FTO/TiO_2. Both these contacts would be placed either side-by-side for an Interdigitated Back contact solar cell configuration or spatially separated by insulating layer like Al_2O_3 or SiO_2 thin-film in a Quasi- Interdigitated back contact solar cell. Since the perovskite is the final layer to be deposited during device fabrication, any losses through parasitic light absorption by the top contact are also avoided and damage to the photoabsorber during subsequent fabrication steps like evaporation of metal electrode is eliminated. Moreover, the shadowing effect of device electrodes is avoided resulting in 100% active area utilization and higher power density in back-contact solar cells as compared to conventional sandwich configurations.

Self-Trapped Excitons mediated Energy Transfer to Sm^{3+} in $Cs_2AgIn_{(1-x)}Sm_xCl_6$:Bi Double Perovskite Nanocrystals

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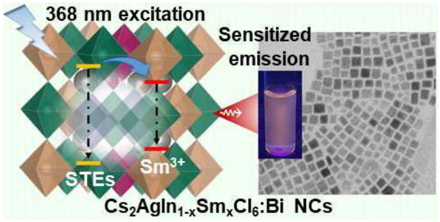
Incorporation of Lanthanide ions (Ln^{3+}) in lead-free halide double perovskites has become an excellent strategy to overcome the challenge of weak photoluminescence. However, the excitation energy of Ln^{3+} doped $Cs_2AgInCl_6$ being too high (~250-290 nm) limits its direct excitation by commercial UV light emitting diodes (≥ 365 nm). To overcome this challenge, we employed sensitization technique by codoping Bi^{3+}(~1%) to induce the emission of Sm^{3+} at much lower excitation energy in Sm^{3+}-Bi^{3+} co-doped $Cs_2AgInCl_6$ DP nanocrystals (NCs). Spectral analysis shows that trace amount of Bi^{3+}(~1%) doping provides enhanced dual emission of self-trapped excitons (STEs) and four characteristic emissions of Sm^{3+} assigned to $^4G_{5/2}$ to ^6H_J (J = 5/2, 7/2, 9/2, and 11/2) transitions. We propose a luminescence mechanism to explain the energy transfer pathway in the synthesized system. Our study demonstrates that Bi^{3+} can efficiently sensitize Sm^{3+} to modify the optical properties of lead-free DP NCs to expand their luminescence application.



Sm^{3+}-Bi^{3+} co-doped $Cs_2AgInCl_6$ DP NCs luminescence

Keywords: Self trapped exciton, energy transfer, ultrafast transient absorption, lead free perovskite

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Synthesized and analysis of $MAPbI_3$ for sensing applications

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Abstract

Here, we have synthesized methylammonium based metal halide perovskites (MHP) i.e., $MAPbI_3$ using methylammonium iodide and lead bromide at room temperature under certain experimental conditions. Synthesized $MAPbI_3$ has been confirmed through different morphological and spectroscopic techniques. Afterward, evaluation on optical properties of $MAPbI_3$ have been made in different solvents using emission spectroscopy. Based on excellent optical properties of $MAPbI_3$ in hexane, we have explored for nitrobenzene sensing applications.

Keyword: Perovskite, nitrobenzene, detection

$Cs_2(Na_xAg_{1-x})BiBr_6$ Nanocrystals: A New Class of Lead-Free Alloyed Double Perovskite with Tunable Band Gap

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Lead-free halide double perovskites have become champion photoactive semiconductors for their applications in optoelectronic devices. $Cs_2AgBiBr_6$ is a well-studied double perovskite, it absorbs in visible region and have indirect band gap due to which it is weakly photoluminescent. Herein, we describe the synthesis of a series of $Cs_2Na_xAg_{1-x}BiBr_6$ (x = 0, 0.25, 0.5, 0.75, 1) alloyed double perovskite nanocrystals. This synthesis provides useful way to make new materials with enhanced photoluminescence and tuneable band gaps by alloying an alkali metal (Na) into $Cs_2AgBiBr_6$. The tuning of bandgap has been further explored by electronic structure calculation under the framework of density functional theory (DFT). The electronic structure calculation confirms that the increase in bandgap is due to reduction in Ag contribution near valence band maxima (VBM) on incorporation of Na in place of Ag. These alloyed double perovskites are potential candidates for making high performance photodetectors.

Morphological and electrical studies of methylammonuium(MA)-free inverted perovskite solar cells

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Abstract:

One of the most promising substitutes for cutting-edge silicon in the production of low-cost solar cells is hybrid organic-inorganic metal halide perovskite. Currently, Perovskite solar cell have higher power conversion efficiency(PCE) greater than 20% with complex compositional and bandgap engineering contain bromine(Br) and thermally unstable methylammonium(MA) molecule. Therefore, avoiding Br and especially MA can lead to more optimal bandgap stable perovskite. Thus, the MA free perovskite solar cells have attracted a great deal of attention owing to the optimal bandgap towards the Shockley-Queisser optimum and the improved thermal stability of $FAPbI_3$-based perovskite. However, at lower temperatures, $FAPbI_3$ perovskite exhibits the unstable photoactive phase. A small proportion of inorganic cation cesium(Cs) was incorporated in FA to stabilise the $FAPbI_3$ photoactive phase. In this work, we investigate the phase and morphology of the photoactive $Cs_{0.1}FA_{0.9}PbI_3$ perovskite structure and fabricated a planar p-i-n based perovskite solar cell which display PCE 14.57% with an open-circuit voltage(V_{OC}) of 923.5mV. Further, photophysical and electrical characterization has to be done to obtain an indepth study of the defects originated during the perovskite crystallization process.

Keywords: MA free perovskite, compositional engineering, morphology, defects.

Fabrication and characterization of Ag doped ZnO TCO

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Abstract: Transparent conducting oxide have been widely used in optoelectrical devices such as electrode material in thin film solar cell because of their low resistance electrical contact. TCO has wide variety of applications such as in photovoltaics, display panels and touch screens.

Among all the ITO exhibit the properties of low resistance and high transmittance but due to shortage of the indium it become very costly to use it. ZnO has come out as best substitute of ITO. As Zinc is present in ample amount than indium. ZnO is a direct band gap semiconductor which is of much interest because of its properties which include wide bandgap (3.37 e V), large exciton binding energy (~ 60 m V). Also, ZnO is of non-toxicity and of low cost. It has a very good transparency in visible region. Undoped ZnO are n type in nature because of its local defects because of oxygen vacancies and zinc interstitials. ZnO has been doped with many group 3A metal group impurity such as Al, Ga and In to increase its properties, but as the impurity concentration is increased in the ZnO gets mobility compromised. To increase electron concentration large number of donor impurity are added to ZnO they turn to positively charge defect and decrease the electron mobility by scattering free electron. To overcome this Ag nanoparticles are added to ZnO because they lead to the p type conductivity due to increase in acceptor level.

Sol gel method has advantages over the other method such as low cost, simplicity and versatility of its experiment procedure. It can be used in production of large area and that too homogenous. The aim of this work to is to develop TCO that is low cost and eco friendly that can be used in various photovoltaic application such as solar cells, photodetectors and many more. Ag NPs are biosynthesised from *Moringa oleifera* aqueous leaf extract. These green synthesised nanoparticles are gaining their popularity because of their various properties like low-cost synthesis techniques and non-toxicity.

Keywords: TCO,Biosynthesised Ag NPs, *Moringa oleifera leaf extract.*

Study of structural properties of rare earth type perovskite titanium oxide for photocatalytic application

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Abstract

Perovskite materials exhibits broad range of structural, electronic and magnetic properties, which are widely used for various application. Impregnation of rare earth metal in perovskite matrix will enhance the physiochemical property also their photocatalytic properties. The compounds such as $PrTiO_3$, $PrSrTiO_3$, $PrCaTiO_3$ were synthesized and prepared by facile combustion method. The as-prepared samples are calcined and analysed for XRD, FTIR and FESEM analysis. XRD (X-Ray Diffraction) confirms the crystalline size, lattice constant and unit cell of the sample. All the sample shows well developed peaks proving the crystalline nature of synthesized rare earth doped perovskite compound. The various stretching and bending vibrational modes were confirmed by FTIR (Fourier Transform Infrared Spectroscopy) analysis. The vibrational frequency of various stretching band of OH group, C=O group formation, with their corresponding metal oxide bond were analysed in the range of 0-4000 cm^{-1}. FESEM (Field Emission Scanning Electron Microscope) of $PrCaTiO_3$ shows flake-like structure, whereas $PrTiO_3$ and $PrSrTiO_3$ are agglomerated cluster were observed. The UV analysis shows the quantitative analysis of the chemical substance present in the sample were studied. From these analysis, $PrCaTiO_3$ compound exhibits better results in physical characterization. Hence, the obtained compounds are suitable for dielectric studies which can be further extended for photocatalyst application.

Keywords: perovskite matrix, metal oxide bond, dielectric studies, photocatalyst.

Elucidating the effect of surface passivation on crystal growth and charge carrier relaxation dynamics in a lead-free double perovskite microcrystals

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Abstract: Layered double perovskites ($A_4B^{II}B`_2^{III}X_{12}$) have drawn attention for the photovoltaic application as an alternative for lead halide perovskite due to their benign character and other physical properties. These perovskites exhibit appreciable photothermal stability. $Cs_4CuSb_2Cl_{12}$ (CCSC) offers facile synthesis methods, is stable to heat, light, and humidity, and has a suitable bandgap for optoelectronic applications. We performed the excited state dynamics of CCSC microcrystals (MCs) and explored the relaxation pathways at different excitation wavelengths, above/near/below the absorption maxima. However, the nature of defect states and how they affect the dynamics of charge carriers in CCSC MCs remains unclear.

To this end, using the solution-processed method we have synthesized bare and ligand-capped CCSC MCs. Our studies revealed that in the presence of surfactant, the growth of the crystals is not irregular but takes a particular (circular) shape. The surfactants passivate the surface trap states. Since trap states play a role in the charge relaxation and transfer process. Using femtosecond transient absorption spectroscopy, we further studied the effect of surfactants on charge carrier dynamics. This analysis shows the presence of deep trap states in the CCSC MCs which can be passivated using suitable surfactants to make it more suitable for photovoltaic application.

Keywords: $Cs_4CuSb_2Cl_{12}$ microcrystals, surfactants, defect states, femtosecond transient absorption spectroscopy, charge carrier dynamics.

The sharp Blue and Green Emission in Eu-doped $CsPbBr_3$ for the Optical Applications

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Abstract: Inorganic halide perovskites (IHPs) have provoked intense research because of their superior stability, excellent optoelectronic properties, cost-effectiveness, and striking optoelectronic applications.[1] Recently, the doping of lanthanide ions in IHPs has opened new avenues, particularly for emerging applications like NIR and white light emitting diodes, NIR emitters, NIR camera, optical temperature sensing, optical data encoding, etc. Besides, lanthanide doping has also improved the stability (thermal, photo, and phase), structure and optical properties of IHPs significantly, which has resulted in improved device performance.

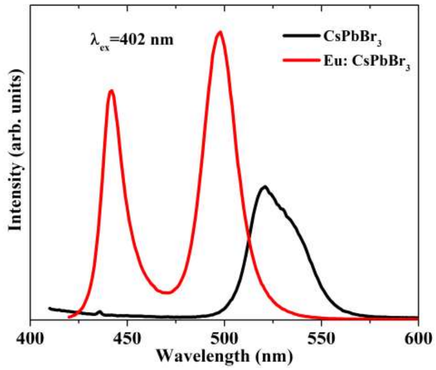

Figure 1. The emission spectra of $CsPbBr_3$ and Eu-doped $CsPbBr_3$ QDs (excitation wavelength is 402 nm).

Here we have synthesized the Europium (Eu) doped-$CsPbBr_3$ quantum dots (QDs) using hot-injection method. For the confirmatory text we performed various characterizations such as ultraviolet–visible absorption, photoluminescence, X-ray photoelectron spectroscopy of the sample.[2-4] The photoluminescence spectra of the $CsPbBr_3$ and Eu-doped $CsPbBr_3$ recorded by using 402 nm excitation light are shown in figure 1. The $CsPbBr_3$ QDs shows the emission peak at 521 nm and Eu-doped $CsPbBr_3$ QDs shows emission peaks at 442 and 498 nm. The results are good agreement with previously published reported. In Eu-doped $CsPbBr_3$ QDs, the emission peak at 442 is due to the Eu-ion and 498 nm peak is from the $CsPbBr_3$ host. It is observed that the emission peak due to the host shift towards lower wavelength on doping Eu-ion. At the same time intensity of the emission peaks also increased due to site symmetry breaking upon the Eu-ion doping into the $CsPbBr_3$. The results show that this material can be explored for different optical applications.[5]

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Keywords: Inorganic halide perovskite, Lanthanide, Quantum dotes, Blue emission, Optical application.

Development of double perovskite Ti-doped La_2NiMnO_6 for magnetocaloric application

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Double perovskites are becoming an important research topic due to their intriguing magnetic properties coupled with electric fields. As the focus of invension of new energy materials which as renewable in nature has taken a speed, the rare earth manganites possess most of the qualities to become a new energy material for cooling purpose. The magnetocaloric effect exhibited by these materials finds application in many energy devices such as refrigerator, cooler etc. The double perovskite structure of rare earth manganites helps in attaining the goal of becoming successful magnetic refrigerant. In this work, Ti-doped La_2NiMnO_6 was synthesized using solid state reaction method. The Ti-doped La_2NiMnO_6 were studied for their structural, magnetic and magnetocaloric properties. The PXRD analysis confirms the monoclinic structure and p21/n(14) space group of Ti-doped La_2NiMnO_6. The space group, bond angles, lattice parameters were derived from the data obtained after Rietvald refinement of the XRD diffraction pattern. The temperature dependence and field dependence magnetic properties were evaluated using SQUID-VSM. The exhibition of magnetocaloric properties were suggested by the presence of second order transition in the temperature dependent magnetic measurement. The magnetic entropy with respect to the Magnetocaloric effect of Ti-doped La_2NiMnO_6 was derived and studied in detail.

Keywords:
Double Perovskite; Solid state reaction; Rietveld refined XRD; Doping; Magnetocaloric effect:

Stability Enhanced Environment-Friendly Bismuth Halide Perovskite for LED applications.

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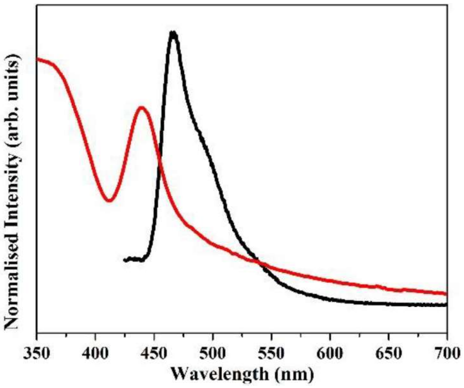
Lead halide perovskites (HPs) have gained tremendous popularity in the past decades because of their excellent properties and wide range of applications. But the presence of lead makes this amazing material toxic and unhealthy for the environment and human lives. Lead-free HPs are comparatively less toxic and more stable. The photoluminescence quantum yield is up to 80% which is quite good for many optoelectronic applications. Bandgap engineering and varying the halide composition spreads the application range from photovoltaics to LEDs to detectors and sensors. Because of their less toxic nature, they can also be used for biomedical applications (like bioimaging).



Here $Cs_3Bi_2X_9$ (X=Cl, Br, I) nanoparticles were synthesized by hot injection method. UV-absorption and PL spectra of synthesized $Cs_3Bi_2Br_9$ nanoparticles shown in the figure are in good agreement with the previously reported work. UV spectrum shows a sharp absorption in the blue region peak at 440 nm. The photoluminescence (PL) spectrum of the $Cs_3Bi_2Br_9$ nanoparticles is recorded by 440 nm excitation. PL spectrum shows a sharp emission peak centred at 465 nm. The narrowband PL emission observed is suitable for LED applications. We have also observed the emission colour tunability by changing the halide composition from Cl to Br to I. Other optical properties of all the synthesised $Cs_3Bi_2X_9$ (X=Cl, Br, I) have been also analysed. Results show that the material can be used for colour LEDs and other optical applications.

Keywords: Lead-free perovskite, nanoparticle, colour tunability, LEDs.

Field and path induced magnetization switching and spin reorientation phenomenon in Ce substituted $SmCrO_3$

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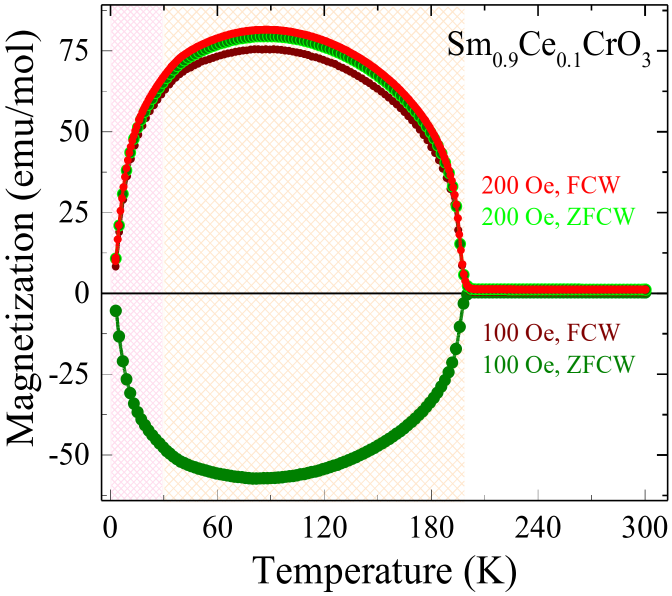
Abstract: Rare earth perovskite chromites with *Pbnm/Pnma* space group of slightly distorted orthorhombic crystal structure exhibit quite intriguing magnetic phenomena such as bipolar switching of magnetization and spin-reorientation phenomena which have direct application towards thermo-magnetic switches, volatile magnetic memory, thermally assisted-MRAM, thermomagnetic power generation etc., [1-3]. In this work we present the field driven magnetic switching and spin reorientation of the Ce substituted $SmCrO_3$ which were synthesized using standard solid state reaction method. The single phase nature of the compound and its electronic structure has been probed by X-ray diffraction and X-ray photoelectron spectroscopy, respectively. Cerium substitution at Sm sites lead to a significant enhancement in the antiferromagnetic Néel temperature (T_N to 202 K) with G-type Γ_4 (G_x, A_y, F_Z) spin configuration as compared to pristine $SmCrO_3$ which shows T_N ~191 K accompanied by a spin reorientation temperature (T_{SR}) at ~ 33 K with an altered magnetic phase Γ_1 (A_x, G_y, C_z) along with the high temperature Magnetic-compensation point (T_{Comp}) ~ 200 K (see Figure). Such intersting feature make the Ce-$SmCrO_3$ as a perfect candidate for aforementioned applications. In the present case Cr^{3+} induced internal field (H_{int}) below T_N which aligns the rare earth Sm^{3+} and Ce^{3+} antiparallel and parallel to the external applied field (H_{DC}) under zero-field cooled warming (ZFCW) and field cooled warming (FCW) condition respectively. The rare earth sublattice magnetization intensifies the anti-parallel component resulting the magnetization switching below T_{Comp}. Such intriguing feature lies in-the field dependence magnetization switching as H_{int} fails to hold the antiparallel moment and the negative magnetization vanishes (for H_{DC} = 200 Oe) whereas it persists upto H_{DC} = 100 Oe under ZFCW protocol. The T_{SR} originates as a result of competing interaction between H_{DC} and net magnetic moment (M_{Net}) with positive Zeeman energy which abruptly switches to negative magnitude (from $\theta = 0$ to Π) resulting a first order phase transition.



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Keywords: Perovskites, Antiferromagnetism, Magnetization Switching, Spin-reorientation.

Defect Passivation with Multifunctional Fluoro-Group-Containing Organic Additives for Highly Efficient and Stable Perovskite Solar Cells

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Abstract: Passivation of defects with functional organic molecules is one of the best strategies to improve the efficiency and stability of perovskite solar cells (PSCs). Herein, two fluorinated organic additives have been utilized to passivate the $CH_3NH_3PbI_3$ perovskite film and study their effects on PSC device performance. The two additives, pentafluoropropionic acid (PFPA) and heptafluorobutanoic acid (HFBA), contain a single carboxylic acid and varying fluoro functional groups. The interaction of these additives with the perovskite was first confirmed by the density functional theory and X-ray photoelectron spectroscopy, and thereafter, PSCs with a p–i–n architecture were fabricated with and without the additives. The champion device has displayed power conversion efficiency of over 20% for the PFPA-modified perovskite. Furthermore, the improvement in charge transport and reduced recombination as a result of the passivation of defects in perovskite are well-studied using various photophysical and impedance studies. Lastly, significant enhancement in ambient stability compared to the pristine device without any additive is observed with the incorporation of fluorinated additives.

Evidence of Short-Lived High Energy Emissive State in Lead-Free $Cs_3Cu_2I_5$ Nanorods

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Abstract: Copper halide perovskites show large stoke-shifted photoluminescence (PL) originating from self-trapped exciton (STE). However, STE emission in materials is always in a competitive relationship with band-to-band emission. But copper halide perovskites show only STE emission which is surprising. In this work, we have investigated the possibility of the presence of band-to-band emission in the $Cs_3Cu_2I_5$ perovskite nanorod. The $Cs_3Cu_2I_5$ was synthesized through the hot injection process with oleylammonium iodide as the ligand which shows a broad PL centered at 445 nm with PLQY of 81%. The PL transients at different wavelengths of the emission spectrum reveal the presence of a very short lifetime component in the order of ~0.5 ns at the blue edge of the emission along with STE component (~500 ns). The time-resolved emission spectral analysis from this experiment further reveals the presence of a high emissive energy state in the ~360 nm region in the early time originating probably from the band-to-band recombination. The absence of this PL band in steady state is may be due to the huge difference in the lifetime with the STE band. This evidence of a high-energy emissive state in the $Cs_3Cu_2I_5$ system is unique and will certainly enlighten the photophysics involved.

Keywords: Copper halide perovskite, Self-trapped exciton, Time-resolved emission spectra, Band-to-band transition.

The effect of halogenated spacer cations on structural symmetry-breaking in 2D halide double perovskites

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Abstract: Non-centrosymmetric materials can be used in optoelectronic applications that effectively separate photogenerated charge carriers (electrons and holes). In the past decade, however, halide perovskites have shown extraordinary photovoltaic performance due to their tunable materials/optoelectronic properties. Layered halide perovskites, in two-dimensional form, crystallizes in non-centrosymmetric space groups and show bulk polarization. Herein, we present a strategy to introduce above-room temperature non-centrosymmetry into two-dimensional halide double perovskites ($A'_4M'M''X_8$) using a halogenated A'-site organic linker, 3-chloro/ bromo propyl amine. These crystals exhibit anisotropic polarization with three orders of magnitude variation between different crystallographic axes. The non-centrosymmetry is further confirmed by piezo-force microscopy studies and its role in the thermal and optical properties was investigated.

Keywords: Non centrosymmetric, Anisotropic, Piezoelectric, Distortion, Layered halide perovskite.

Compositional engineering and surface passivation for carbon-based perovskite solar cells with superior thermal and moisture stability

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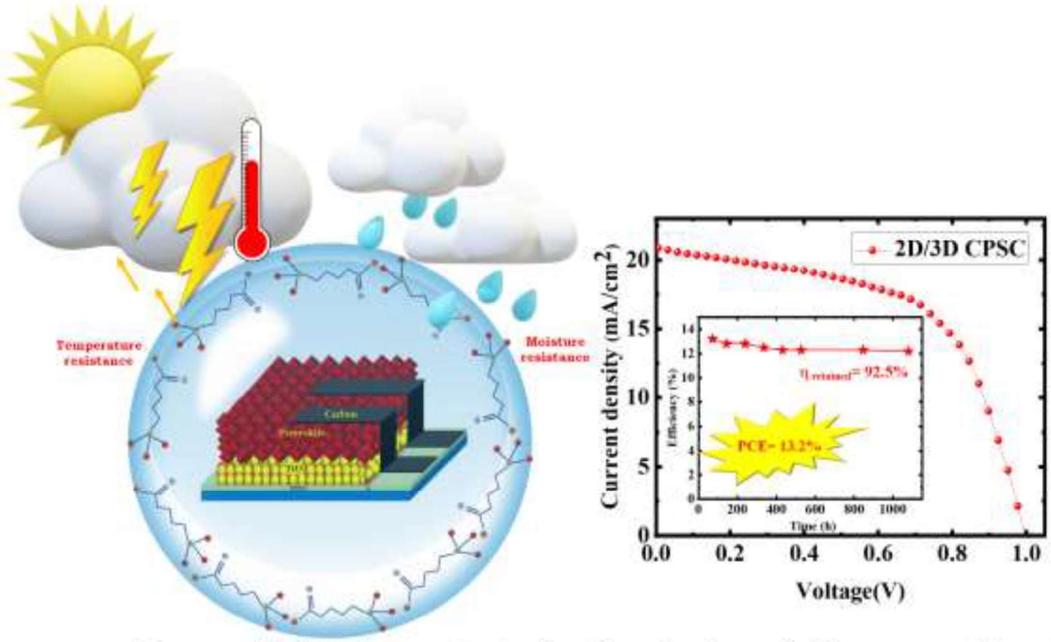
Abstract: The inherent stability of perovskite absorbers towards environmental factors is a major limitation towards commercializing perovskite solar cells (PSCs). In this regard, $MaPbI_3$ (MAPI) is engineered to attain thermal stability by incorporating Guanidinium iodide (GuI) and moisture stability by surface passivation using 5- amino valeric acid iodide (5-AVAI). The surface passivation of Gu modified MAPI, hereafter termed as GUMAPI, exhibits a 2D/3D perovskite interface, which, facilitates perovskite to attain high moisture and temperature stability. Various concentrations of 5-AVAI are used as the surface passivator. The stability of the surface-modified Gu doped MAPI films is studied thoroughly using time-dependent water contact angle measurements, in-situ temperature-dependent XRD analysis, and XRD studies of aged perovskite films under ambient conditions. 1AV films exhibit excellent temperature (>150°C) and ambient stability (>59 days) when compared with control perovskite films (GUMAPI). The stability and performance of these perovskite films in a carbon-PSCs (CPSCs) architecture are evaluated by studying the current-voltage characteristics and assessing the device performance at various intervals. The 1AV-based CPSCs exhibit performance surpassing the control (GUMAPI) devices. A 9.0% increment is observed in the 1AV-based CPSCs compared to the GUMAPI-based CPSCs with an efficiency of 13.2% and a T_{80} lifetime of 93.2% without encapsulation.



The synergetic effect of compositional engineering and surface passivation was successfully used to engineer perovskite films stable to moisture and temperature

Semi-transparent Photovoltaic Devices incorporating Oxide-Metal-Oxide-based Top Transparent Electrodes

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Abstract: This study deals with the optimization of the stack of a semitransparent perovskite solar cell to get the best trade-off between device transparency and performance. Using optical modeling, 64 different combinations of top transparent electrodes (TEs) based on the oxide-metal-oxide (OMO) structure were studied. An OMO-TE consisting of NiO/Ag/SnO_2 having maximum average visible transmittance (AVT), was then studied into an *n-i-p* geometry device consisting of SnO_2, Spiro-OMeTAD, and $MAPbI_3$ as the electron transport layer (ETL), hole transport layer (HTL), and light absorbing layer, respectively. The complete device stack was then optimized considering the thickness as the varying parameter. To get balanced results, the ratio concept of the overcoat-to-undercoat layer of OMO-TE is introduced. It has been found that for a ratio of 1.17, a maximum J_{SC} of 4.34 $mAcm^{-2}$ is obtained, while for a ratio of 0.78, a maximum AVT of 21.55% is obtained. In this manner, a region is defined considering the maxima of J_{SC} and AVT of the device as the extreme point to get the best trade-off between J_{SC} and AVT of the device, as shown in Figure 1. At last, it is shown that an optical spacer after OMO-TE can enhance J_{SC} by 115%.

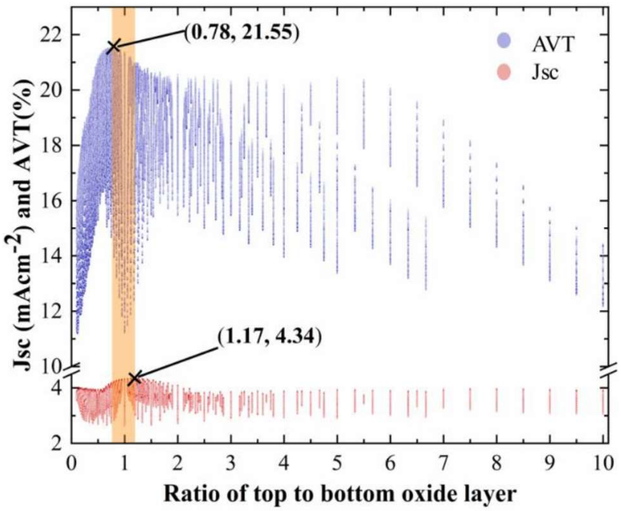

Figure 1: Variation in J_{SC} and AVT of the device as a function of ratio of top to bottom oxide layer of OMO stack. Purple color dots represent AVT, and red color dots represent the J_{SC} of the device. The values in the parentheses represent the ratio and the corresponding best AVT or J_{SC}.

Keywords: Semi-transparent, Perovskite Solar Cells, Transparent Electrode, Optical Spacer, Optical Modeling

Tuning Crystal Plane Orientation in Multijunction and Hexagonal Single Crystalline $CsPbBr_3$ Perovskite Disc Nanocrystals

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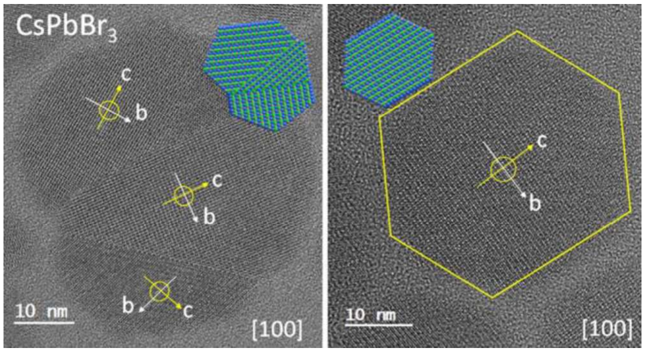
Abstract: Two-dimensional-shaped $CsPbBr_3$ platelet nanocrystals are widely studied for their bright high energy emission and self-assembly. These nanostructures are in orthorhombic phase, Single crystalline square shaped, and have the vertical axis [001] perpendicular to the basal plane. In contrast, herein, multijunction and hexagonal single crystalline 2D discs of $CsPbBr_3$ are reported to have all their vertical axes [100]. These are obtained by using the perovskite derivative of tetragonal Cs_3MnBr_5 as the parent material and subsequent B-site Pb(II) introduction in the presence of phenacyl bromide at different reaction temperatures. At low temperature, multijunction discs having random orientations of two horizontal axes [010] and [001] from one to another segment are observed. Orientations of planes remained random as both coherent and incoherent twin planes were observed at their boundaries. Analysis suggested that the crystal nature of parent Cs_3MnBr_5 and temperature-dependent variation in the rate of Pb(II) insertions determined the nature of discs having randomly oriented or static planes in the entire nanostructure. These hexagonal single crystalline and segmented multijunction $CsPbBr_3$ discs remain unique among 2D perovskites nanostructures, and their formation mechanism indeed introduced new fundamentals of the crystallization process of these emerging energy materials.



Keywords: Nanoplatelet, Lead-halide perovskite, Crystal plane rotation, Hexagonal , Multi-junction

Enhanced and tunable emission from distorted $Cs_2Ag_{0.5}K_{0.5}InCl_6$ double perovkite by La^{3+} doping

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Abstract:

The fluorescence properties of the double perovskites (DP, $Cs_2AgInCl_6$) can be tuned by incorporation of external atoms or creating defect states. This could create luminescent active centers in the perovskite host material or distort the perovskite structure, which have proportional effect in improving the photoluminescence. Incorporation of K^+ ions into DP induces short range structural disorder and multiphase formation. Further, La^{3+} doping on distorted double perovskite ($Cs_2Ag_{0.5}K_{0.5}InCl_6$) helps to enhance and tune the emission spectrum. Rare earth ions such like La^{3+} is spectroscopically innocent but it can reduce the energy of the whole system by reducing the conduction band from the the hybrid effect of La 6s. We examined the structural and electronic band effects of La^{3+} doped distorted double perovskite systems using theoretical calculation methods and optical characterisation techniques. XRD and Raman spectroscopy analysis confirms that the distorted DP structure and photoluminescence measurements shown that while La introduced into the distorted DPs giving the very broad emission i.e. FWHM incresed from 170 nm to 215 nm with PLQY of 37 %. These fully inorganic La^{3+} doped distorted DP compound can be deomonstrated as a bright emissive material for stable lighting applications.

Keywords: Double Perovskite, Photoluminescence, Distorted perovskite, Jahn-teller distortion, Broad emission.

Buried Interface Passivation of Perovskite Solar Cells by ALD Al_2O_3

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Abstract: Despite having long excited carrier lifetimes and high mobilities in hybrid halide perovskite materials, the conventional (n-i-p) devices witness significant interfacial non-radiative recombination losses that are little understood but limit its radiative efficiency and the overall open circuit potential. Here, we reveal that the process of spiro-OMeTAD coating on perovskite gives rise to buried defect states, detrimental to devices' operational stability. We subsequently report a method to passivate these deleterious buried defect states by atomic layer deposition of Al_2O_3 through controlled precursor dosages on fully functional devices. The reported passivation technique results in; (a) an increase in the efficiency primarily due to an increase of V_{OC} by ~ 60-70 mV, and consequently, (b) enhanced photoluminescence and higher electroluminescence quantum efficiency, (c) overall device operational (MPPT) stability under ambient and, exclusively, even under high vacuum (> 300 hrs.), which is otherwise challenging.

Keywords: Perovskite solar cell, ALD-Al_2O_3, Defect passivation, Stability,Vacuum

Investigating the property of Water-Driven Lead-Free Stable Inorganic Halide Double Perovskites

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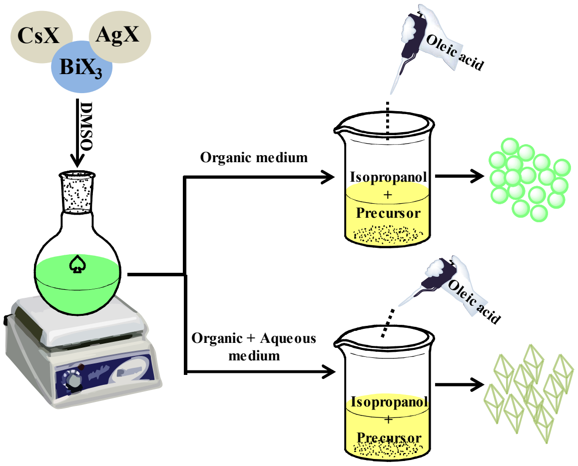
Abstract: Lead-free halide double perovskite materials, $A_2BB'X_6$ (where A, B, and B′ are cations and X is a halide anion) have achieved considerable attention in the field of optoelectronic devices due to their high thermal along with the moisture stability and less toxicity as lead halide perovskites suffer from the stability and toxicity issues which inhibit them to be commercialized.[1,2] Therefore, the synthesis of low-cost and stable perovskite materials is the main focus of the perovskite family nowadays. Herein, we have synthesized lead-free $Cs_2AgBiCl_6$ and $Cs_2AgBiBr_6$ double perovskite microcrystals in both organic and a mixture of the aqueous-organic medium (**Scheme 1**). Our studies are not only eradicating the toxicity of lead but also explored towards the stability of perovskite materials in the aqueous medium. The morphology of the materials is investigated using SEM and TEM imaging along with the enhancement in emission peak by increasing the content of water.



Scheme 1. Schematic representation for the synthesis and morphology of microcrystals.

Keywords: Lead-free double perovskite, water stability, morphology, fluorescence.

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Self-healing of the sputter induced damages in halide-perovskite photovoltaic devices

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Organic-inorganic halide perovskites pursue unique self-healing ability, often under the influence of the external inducements. Through this presentation, we show a unique self-healing of the interfacial electronic defects in a multication halide perovskite device under *n-i-p* configuration with sputtered deposited NiO as the hole transporting material. With a combination of spectroscopic and charge-transport studies (both steady-state and transient), We show that the self-curing of the sputter induced damages with time; resulting an increase in the devices efficiency from 4.5% to a steady-state value of 11% within a span of a week to 10 days. We explicitly show the effect of the surrounding ambient, especially the humidity not the oxygen, which essentially acts as the stimuli for the healing mechanism and hence the healing rate can be externally controlled.

Influence of small molecular additive and excess organic cation during $MAPbBr_3$ perovskite emission layer crystallization and their influence on the performance of perovskite light emitting diode devices

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Abstact: Recently metal Halide Perovskites (MHPs) have drawn a lot of interest as a possible alternative soft semiconducting material for next generation optoelectronic devices including solid state light emitting devices. In this contribution, we study the influence of small molecular additive commonly known as TPBi [1,3,5-Tris(1-phenyl-1Hbenzimidazol-2-yl)benzene] and the presence of excess A site cation in $\mathrm{MAPbBr_3}$ (ABX_3) perovskite emission layer fabricated by nanocrystal pinning approach that was earlier introduced by T W Lee and coworkers [1]. Small molecular semiconducting TPBi additive has favourable energetic alignment, resulting in lower charge injection barrier. Consequently, the perovskite LED devices with TPBi additive show lower turn on voltage [2.9 V] compared to Perovskite LED devices with without the TPBi as additive in the emission layer [3.5 V] during crystallization. Further more, we observe presence of excess of MA organic cation during crystallization reduces non-radiative recombination evident from steady state and time resolved photoluminescence decay dynamics experiments.The optimized perovskite LED devices have lower turn on voltage (2.9 V), bright electroluminance of 21370 cd/m^2, improved current efficiency of 15.96 cd/A and external quantum efficiency (EQE) of 3.50 % .

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Keywords: Organic small semiconducting molecule, Nanocrystal Pinning, Defect Passivation, Energy Level alligment, Radiative recombination.

Tuning the Dielectric Properties of Strontium and Calcium Doped Praseodymium Perovskite for Photocatalytic Degradation

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Abstract:

Perovskite materials are gaining interest in various fields like solar cells, magnetic storage devices, photocatalytic degradation etc due to their electric, magnetic, catalytic properties. The incorporation of rare earth elements into perovskite matrix results in physio-chemical change enhances the photocatalytic properties. The rare earth doped perovskite compounds such as $PrMnO_3$, $PrSrMnO_3$ and $PrCaMnO_3$ were synthesized by solution combustion method. The physical characterizations were carried to analyse the formation of the synthesized compounds. XRD result confirms the formation of crystalline structure of the synthesized materials and their crystalline size was calculated. All three compounds exhibit the various symmetric and asymmetric modes of vibrations. Stretching and bending modes of C=O, Mn-O and OH bonds were studied by FTIR. FESEM analysis shows the surface morphology of the prepared compounds. $PrMnO_3$ shows the homogeneous formation of spherical particle. The formation of agglomerated particles in $PrSrMnO_3$ and $PrCaMnO_3$ were observed. The UV analysis shows the quantitative analysis of chemical substance present in the sample were studied. With these results all the three compounds were well suited for photocatalytic application. We will further examine the photocatalytic behaviour of the synthesized materials and the best among them will be used as a photocatalyst for degradation of solid wastes.

Keywords: perovskite matrix, photocatalyst, agglomerated, degradation

Effect of Size of PbSe Nanoparticles on the Optical Properties of $CsPbBr_3$-PbSe Nanoheterostructures

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Manash R. Das,[3] *Pralay K. Santra*,[2] *Dibyajyoti Ghosh*,[1, 4,] *Sameer Sapra*[1,] *

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Abstract.

Nanoheterostructures (NHSs) based on lead halide perovskites (LHPs) and chalcogenide quantum dots have proved to be promising candidate for device applications. However, understanding the defect chemistry at the interfaces of LHPs and chalcogenides is essential to further tune optoelectronic properties. Here, we demonstrate a route for design of $CsPbBr_3$-PbSe NHSs and study the effect of size of PbSe NPs on their optical properties. In this synthesis route, PbSe nanoparticles are formed at an early stage of reaction, over which $CsPbBr_3$ nanocrystals are epitaxially grown. Using this methodology, nearly 3.5-fold enhancement in photoluminescence is achieved, whereas other selenium-precursors which form larger sized PbSe NPs result in negligible PL enhancement. Detailed density functional theory calculations suggest that PbSe NPs are responsible for passivating the surface defects that consequently enhance PL intensity. Furthermore, resulting $CsPbBr_3$-PbSe NHSs demonstrate enhanced stability in presence of water and do not degrade under ambient conditions for several months.

P-Co-Mo Heterojunction Effect towards Hydrogen Evolution Reactions

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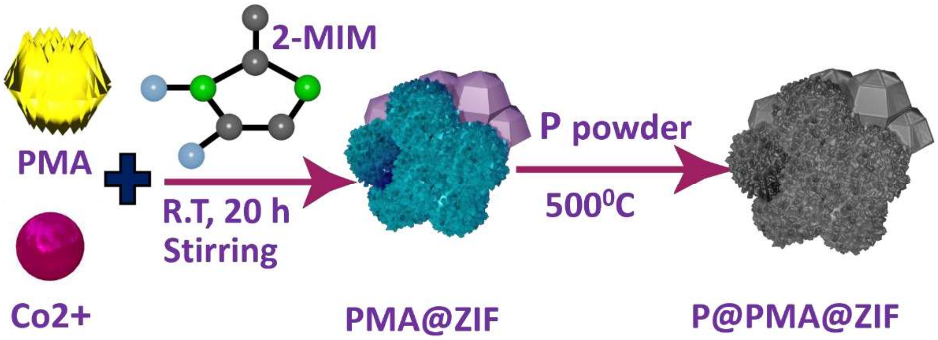
Abstract

Rational design of efficient hydrogen evolution reaction (HER) electrocatalysts for mass production of hydrogen via electrochemical water splitting is a challenging but pressing task. It can be a feasible choice to use noble-metal-free electrocatalysts.[1] First principle calculation demonstrates that introducing Hetero atom linkage with a high-valent transition metal into a metal-organic framework lattice triggers the in situ electron donation from metal-organic framework to transition metal to hetero atom and consequently reduces the energy barrier for the HER.[2]

Transition metal dichalcogenides are gaining much interest in the energy conversion/storage sector due to the 2D nature and conductivity of the materials. However single transition metal dichalcogenides are not stable, preventing their practical usage in real devices.[3] Thus, a metal -organic-framework host and a transition metal-based redox guest with the addition of hetero dopant create a remarkable electrocatalytic performance for hydrogen production from both acidic and basic solutions. [4] Herein, we demonstrate the synthesis of binary metal dichalcogenides (Co-Mo-P) via carbonization of zeolitic imidazolate framework (ZIF-67) metal-organic framework encapsulated with phosphomolybdic acid (PMA@ZIF-67).



Scheme1. Schematic illustration of Phosphomolybdic acid confined on ZIF-67 and doping of P.

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Study for deposition coating technique in perovskite based solar cell.

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Abstract: In this investigation discussed the study on brush coating and spin coating technique. Present study investigated low-cost deposition method of ETL. Precursor solution prepared by 50 ml of iso-propyl alcohol, 4gm of pure stannic oxide, 1gm of urea and 5ml of HCL. The solution stirred at 300 RPM for 3hours and heated at 60°C for 2 hours. Fibril brush used for brush coating and thermal annealing maintained using hot plate for1minute. Spin coating performed at 1000 RPM for 10 second. In E-DAX characterisation tin and oxygen highly traced in both coating methods. From XRD data observed that brush and spin coated samples were respectively higher and low intensity peak detected. The grain and surface texture of SnO_2 films are investigated using a SEM. It is found that that brush coated films are roughly arranged on the other hand spin coated sampled obtained uniform surface morphology. Using tauc relation, bandgap of 3.72 and 3.71 eV were observed brush and spin coated sample, respectively, it shows that brush coated sample have enhanced bandgap. The XPS data confirmed that the electronic transition in Sn3d state.This characterization data conformed that brush coating technique is ideal method for deposition of perovskite based solar cell.

Keywords: Max 5 keywords

Ultra-Fast Preparation of Organic-Inroganic Metal Halide Perovskite Structured $CH_3NH_3PbI_3$ (MAPI) for Improved Nonvolatile Resistive Switching Memory Performance

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Abstract: Ultra-fast, sustainable microwave-solvothermal (MW-ST) technique was adopted to synthesize organic–inorganic methyl ammonium lead iodide ($CH_3NH_3PbI_3$, MAPI) at 120 °C, without requiring any inert atmosphere under high-humid conditions at Pondicherry University located at south-east coastal area of India 65 ± 5% RH and ~28 °C). XRD analysis revealed that highly pure and crystalline MAPI achieved within 10 minutes under MW-ST conditions could remain stable for ~1.5 years. Subsequently, the as-synthesized MAPI powders were dissolved in aprotic solvents (DMF/DMSO) and allowed to recrystallize into thin films using spin-coating *via* a solution-based nanoscale self-assembly process. For application potential of MAPI, nonvolatile bipolar resistive switching (NVBRS) memory devices were fabricated using HfO_2-TiO_2 protected by Al_2O_3 as stacked base-layer for MAPI electrolyte-layer sandwiched between Ag and FTO electrodes. Robust conductive filament (CF) formation was observed owing to prompt heterojunction development between base layer and electrolyte layer in Ag/MAPI/Al_2O_3/TiO_2-HfO_2/FTO configured memory device enabled extremely low operating voltages (SET + 0.2 V, RESET - 0.2 V) and enhanced resistance window ratio (10^5 for $>10^4$ s) compared to pristine MAPI device (± 1 V, 10^2, 10^4 s). The adopted innovative strategies open avenues toward achieving structurally and operationally stable perovskite powders obtained *via* MW-ST at high-humid condition for optoelectronic memory device applications in AI, IoT, and neuromorphic computing.

Keywords: *microwave-solvothermal, nonvolatile bipolar resistive switching (NVBRS) memory devices, organic-inorganic perovskites, RRAMS,conductive filaments, ,*

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Discotic Liquid crystalline based Hole Transporting Material for efficient Perovskite Solar Cells

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Abstract: Renewable energy has attracted global attention to address the global energy and environmental crisis. IAmong 4rth generation photovoltaics Perovskite Solar Cells (PSCs) is emerged as promising, high-efficiency, low-cost solar cells. In the past decade, the PSC's efficiency has risen to > 25% which is comparable to cistalline Silicon. In these PSCs SpiroOMeTADis used as hole tranporting material (HTM) to effectively extract holes from generated charges upon absorption of photon. However, SpiroOMeTAD requires additives to enhance their hole mobility. The use of additives in HTM reduces PSCs stability and increases device complexity. Therefore, new HTMs must prioritise for low cost, stable and device simplicity with improved efficiency.

In this study a new class of discotic liquid crystalline organic semiconductors (HAT4) with good hole mobility of 10^{-2} cm^2/V.s as HTM in PSCs without any additive. Inverted devices were fabricated using HAT4 as HTM in *n-i-p* structure with SnO_2 as electron-transporting layer. An efficiency of 14.3 % (V_{oc} = 1.02 V, J_{sc} = 19.9 mA/cm^2 and FF = 70.5 %) as compared to fully doped SpiroOMeTAD with 16.2% (V_{oc} = 0.88V, Jsc = 23.0 mA/cm^2 and FF = 80 %) was observed which is promising as the cost of HAT4 is miniscule compared to SpiroOMeTAD (Figure 1).

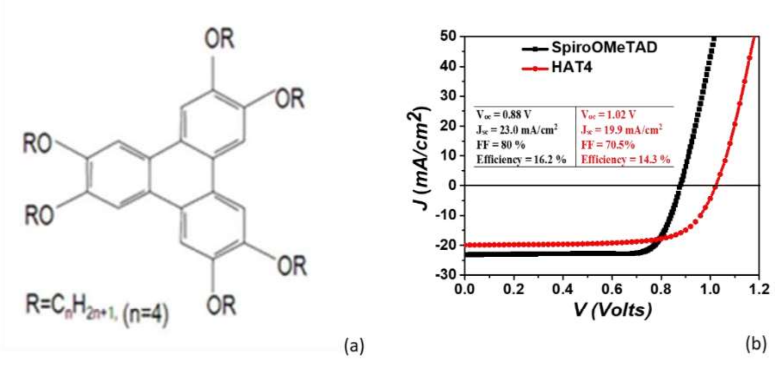

Figure1. (a) Molecular structure of HAT4 and (b) J-V curve for the best performing device with Spiro-OMeTAD (Fully Doped) and HAT4 (Undoped) under 100 mW/cm^2 Illumination.

Keywords: Discotic Liquid Crystals, Perovskite Solar cells, Hole transporting Material, Hole mobility.

Negative Photoconductivity in Lead-Free Perovskite Single Crystals

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Abstract: Recently, halide perovskites have emerged as a promising material for device applications. Lead-based perovskites have been widely explored, while investigation of the optical properties of lead-free perovskites remains limited. Lead-halide perovskite single crystals have shown light-induced positive photoconductivity, and as lead-free perovskites are optically active, they are expected to demonstrate similar properties. However, we report here light induced negative photoconductivity with slow recovery in lead-free Cs3Bi2Cl9 perovskite. Femtosecond transient reflectance (fs-TR) spectroscopy studies further reveal that these electronic transport properties are due to the formation of light-activated metastable trap states within the perovskite crystal. The figure of merits was calculated for Cs3Bi2Cl9 single-crystal detectors, including responsivity (17 mA/W), detectivity (6.23 × 1011 Jones), and the ratio of current in dark to light (~7160). These observations for Cs3Bi2Cl9 single crystals, which were optically active but showed retroactive photocurrent on irradiation, remain unique for such materials.

Scap-1D Performance Analysis of $MAPbI_3$ and $MASnI_3$ Based Pervoskite Solar Cells'

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Abstract:

The software SCAPS 1-D was used in this study to simulate Perovskite Solar Cells (PSCs) with two different absorbing materials and compare their performances. It can be concluded that $MASnI_3$ has the potential to replace $MAPbI_3$ as an absorber material in PSCs. To compare their performances, the thicknesses of the ETL, HTL, and absorbing layers were optimized. To compare their performances, the thicknesses of the ETL, HTL, and absorbing layers were optimized. The simulation results of optimised PSCs revealed that $MASnI_3$ had lower performance than $MAPbI_3$, with $V_{oc} = 0.7945V$, $J_{sc} = 27.95mA/cm^2$, FF =53.99%, and efficiency =12%, which are significantly lower than the PSC with $MAPbI_3$ ($V_{oc} = 1.473V$, $J_{sc} = 14.985mA/cm^2$, FF = 83.68% and efficiency =18.49%) except J_{sc}. However, as mentioned by another researcher, the experimental results showed even lower efficiency, at 6.4%. Despite its lower performance, $MASnI_3$ is more stable than $MAPbI_3$, which is a significant advantage given the toxic nature of lead (Pb). The lower efficiency of $MASnI_3$ could be improved by optimising the bandgap alignment, making it a more promising alternative to $MAPbI_3$. PSCs are an important area of study because they have the potential to revolutionise the electricity generation process, and their applications in flexible electronics and building-integrated photovoltaics are promising.

Keywords: *Perovskite Solar Cells, $MAPbI_3$, $MASnI_3$, ETL, HTL, SCAPS 1D, Simulation.*

Creating defects by copper doping into $Cs_2AgBiBr_6$ and exploring the charge carrier's dynamics using pump-probe spectroscopy

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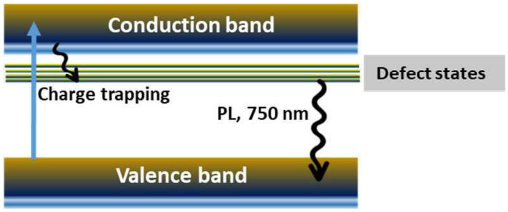
Abstract: Over the decade, inorganic-halide perovskites have become top contenders for next-generation effective LEDs and solar cells. Recently, lead-free double perovskite($A_2B'(III)B''(I)X_6$) nanocrystals have emerged to address instability and toxicity problems associated with lead-based predecessors. The device's performance is however limited by its subpar absorption characteristics, which can be improvised through doping[1]. We have synthesized Cu-doped $Cs_2AgBiBr_6$(CABB) nanocrystals (first time) using colloidal-synthesis approach and performed pump-probe spectroscopic investigations to unravel the underlying charge carrier dynamics. Preliminary studies have confirmed the successful doping of copper ions into CABB crystal lattice. The absorption spectrum shows an enhanced absorption in NIR-region, while fluorescence spectrum implies significant quenching and broadening with copper doping. From PL spectrum, the position of defect states was located at sub-bandgap position. The ultrafast transient absorption (TA) measurements revealed faster recovery for bleach signals(involving bound excitons) in comparison to CABB. It is evident from TA, these sub-bandgap defect states create an extra channel for the depopulation of high-energy bound exciton states. But interestingly, optical pump terahertz probe spectroscopy resulted in higher effective mobility (enhanced absorption leads to more charge carriers) and slower decay trace (charge carriers trapping at defect states) for Cu-CABB. This research provides fresh insight into controlling halide double perovskites for efficient optoelectronic devices like NIR photodetectors.



Keywords: Cu-doped CABB, pump-probe spectroscopy, defect states, charge carriers trapping.

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Synthesis, characterization and excited state dynamics in a lead-free layered double perovskite nanocrystals

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Abstract:

The majority of the world's energy requirements are met by fossil fuels which are limited and are hazardous to human health and to environment. So we must explore non-conventional, eco-friendly, renewable energy sources such as active materials for solar cells. In this regard, perovskite-based photovoltaic technology is the fastest-growing. Its efficiency went up to 24% in just 10 years of research. The primary issue with the previously reported lead-based perovskite is the toxicity due to the presence of lead used as a bivalent cation. This has prompted researchers to explore other non-toxic and more stable substituents to lead halide perovskites for solar cell application.

The discovery of double perovskites (DPs) opened up new possibilities for the production of stable, lead-free perovskites. In this respect, a novel class of DPs $Cs_4CuSb_2Cl_{12}$ (CCSC) has emerged with excellent properties such as facial synthesis, tunable band gap, high stability, high absorption coefficient, long diffusion length, etc. That makes it an auspicious material for solar cell applications.

We synthesized a colloidal solution of CCSC nanocrystals by using hot-injection method. We also performed the essential characterization to explore the physical properties of the material and TGA analysis to check the stability and further studied the charge carrier dynamics using femtosecond transient absorption spectroscopy.

Keywords:

Solar cell, Lead free layred double perovskite , $Cs_4CuSb_2Cl_{12}$ nanocrystals, Excited state dynamics, Transient absorption spectroscopy.

Synthesis and Characterization of Novel Medium and High Entropy Perovskite Oxides

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Abstract

Perovskites, with the chemical formula, ABO_3 where A and B are cations of different sizes, are a class of oxide ceramics which find applications in diverse fields. Many types of elemental and compound doping have been done in perovskites to enhance their properties. However, there is very limited reported in the field of multicomponent perovskites where multiple number of cations are present in the A and/or B sites in equiatomic proportions. In this investigation, an attempt has been made to synthesize and characterize such perovskites. Different rare elements along with sodium were chosen in various combinations for the A-site on the basis of Hume-Rothery and Pauling's rules while titanium was fixed as the B-site cation. The systems were synthesised using the reverse co-precipitation (RCP) method from nitrate precursors for the A-site cations along with an organometallic precursor for Ti. X-ray diffraction (XRD) confirmed that the powders were phase-pure perovskite. The elemental percentage was determined using energy dispersive spectroscopy (EDS). The particle size and morphology were determined using a scanning electron microscope (SEM). The bandgap of the phase pure powders was determined using diffuse reflectance spectroscopy and were compared with the individual titanates.

Keywords: multicomponent, equiatomic perovskites, reverse co-precipitation, bandgap.

Stereochemical Activity of *ns*^{2} Metal Ions & Dopants, Structure-Property Correlation, Host-Dopant & Dopant-Dopant Interaction in Low Dimensional Metal Halide Hybrids

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Abstract: 3D lead halide perovskite has seen a phenomenal research interest in the last decade for applications in photovoltaics and solid state lighting. Their low dimensional counterparts (2D, 1D, 0D), supporting strongly bound excitons, are well-suited for lighting applications. These low dimensional metal halide hybrids show narrow band edge and broadband self-trapped excitonic (STE) emission. In the absence of general guidelines to enhance this broadband emission, structure-property correlation can be beneficial in designing highly emissive materials. In this talk, I will highlight the fundamental factors that control the emissive properties of main group ns^2 metal halide based low dimensional (1D, 0D) hybrids. The mechanism of broad band emission in these low D perovskites, involving STEs and the stereochemical activity of the ns^2 lone pair, will be discussed. I will showcase our current results on multi-metallic halide hybrids incorporating hetero-metallic units that manifest interesting photo-physical properties. Effects of electronic interaction between the metal halide units in such multi-metallic low dimensional hybrids will be highlighted. Mechanism of the electronic cross-talk between the isolated metal halide units in such systems will be discussed. I will conclude the talk with outlook of our current research work highlighting the existing issues in white light emission using main group low dimensional metal halide hybrids.

Keywords: metal halide hybrids, low dimensional, doping, electronic coupling, STEs

Laboratory for Integrated Nano-photonics & Bio-materials
(Satapathi Lab)

Satapathi Lab has wide range of research fields on perovskite materials ranging from fundamental studies such as charge carrier dynamics, structural disorder studies, lattice-vibration, polarons, singlet fission etc. to application such as Photodetectors, X-ray detectors, Solar Cells, LEDs, FETs etc.

In perovskite solar cell field, we are among the leading research labs in india. Our achievement is the fabrication of all air processed and stable perovskite solar cells upto 20% efficiency. We have designed and reported dual solvent elimination method which leads to larger grain size and better crystallinity at room temperature. Recently, we have started fabrication of semi-transparent solar cells for building integration. Building energy consumption accounts for more than a third of world's total energy consumption. Making buildings energy efficient by integrating transparent solar photovoltaic panel into the building fabric is our priority. In addition, we are developing perovskite materials based next generation X-ray detectors for X-ray imaging. Our prototype X-Ray detectors shows higher Sensitivity (400 μC Gyair-1cm^{-2}) at low bias (2 V mm^{-1} Electric field) making it suitable for medical imaging and security surveillance. These X-Ray imagers are portable and low cost.

Moreover, we have a sensor team to develop microfluidics devices-based sensors, optical sensors, electrochemical sensors for nitro-aromatics and biological analytes. We have an expertise in development and fabrication of microfluidic Lab-on-Chip systems using novel 3D-printing based approaches. We have designed and patented microfluidic systems for integrated on-chip asaays and point-of-care diagnostics.

During the last three to four years we have published more than 100 research papers in leading journals of material science. Also, few of our works have been patented and in the process of technology transfer. Recently, our work on perovskite solar cells, X-ray detectors, and sensors have got huge media attention.