Nanomaterials and Molecules: From Spectroscopy to Bioimaging

(NaMoSBio 2026)

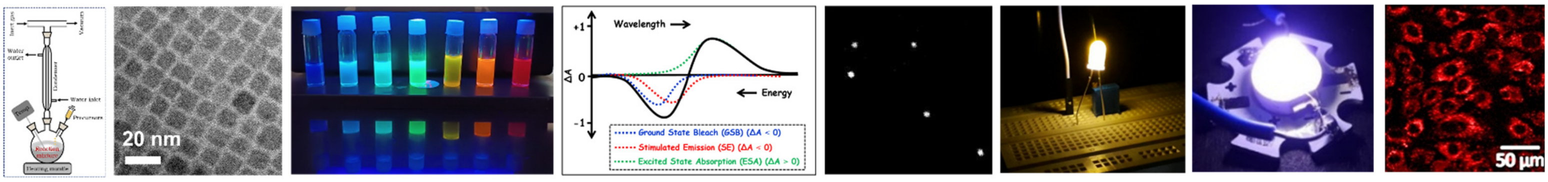
An International Conference

@

IISER KOLKATA

R N Tagore Auditorium, IISER Kolkata

23-26 January, 2026



Nanomaterials and Molecules: From Spectroscopy to Bioimaging (NaMoSBio 2026)

An International Conference @ IISER Kolkata

R N Tagore Auditorium, Indian Institute of Science Education and Research (IISER) Kolkata, India | **23-26 January, 2026**

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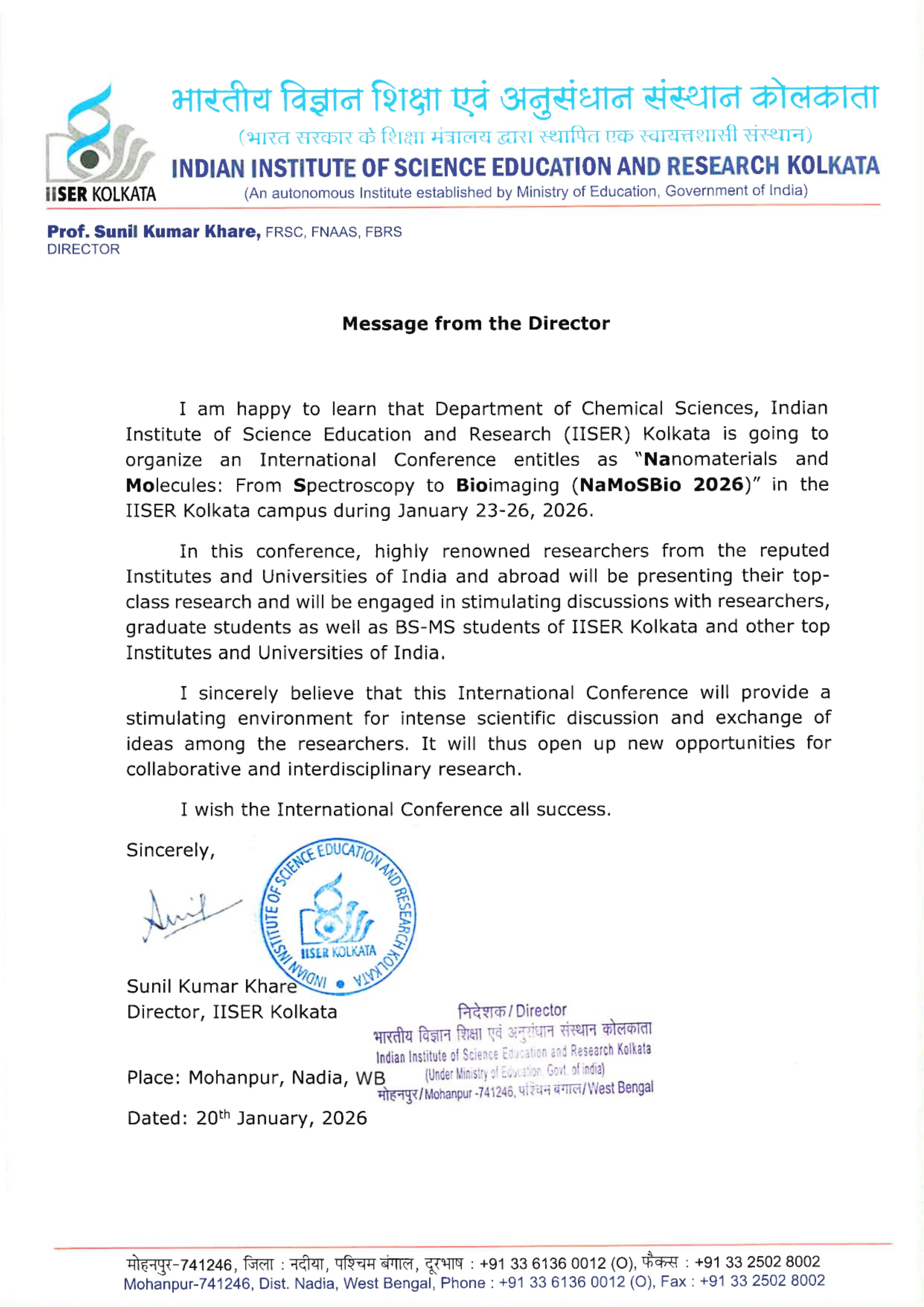
Professor Prasun K. Mandal, IISER Kolkata, India

Co-Convener:

Professor Priyadarsi De, IISER Kolkata, India



भारतीय विज्ञान शिक्षा एवं अनुसंधान संस्थान कोलकाता
(भारत सरकार के शिक्षा मंत्रालय द्वारा स्थापित एक स्वायत्तशासी संस्थान)
IISER KOLKATA
INDIAN INSTITUTE OF SCIENCE EDUCATION AND RESEARCH KOLKATA
(An autonomous Institute established by Ministry of Education, Government of India)

Prof. Sunil Kumar Khare, FRSC, FNAAS, FBRS
DIRECTOR

Message from the Director

I am happy to learn that Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Kolkata is going to organize an International Conference entitles as "**Na**nomaterials and **Mo**lecules: From **S**pectroscopy to **Bio**imaging (**NaMoSBio 2026**)" in the IISER Kolkata campus during January 23-26, 2026.

In this conference, highly renowned researchers from the reputed Institutes and Universities of India and abroad will be presenting their top-class research and will be engaged in stimulating discussions with researchers, graduate students as well as BS-MS students of IISER Kolkata and other top Institutes and Universities of India.

I sincerely believe that this International Conference will provide a stimulating environment for intense scientific discussion and exchange of ideas among the researchers. It will thus open up new opportunities for collaborative and interdisciplinary research.

I wish the International Conference all success.

Sincerely,

Sunil Kumar Khare
Director, IISER Kolkata

निदेशक / Director
भारतीय विज्ञान शिक्षा एवं अनुसंधान संस्थान कोलकाता
Indian Institute of Science Education and Research Kolkata
(Under Ministry of Education, Govt. of India)
मोहनपुर / Mohanpur -741246, पश्चिम बंगाल / West Bengal

Place: Mohanpur, Nadia, WB

Dated: 20th January, 2026

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भारतीय विज्ञान शिक्षा और अनुसंधान संस्थान–कोलकाता
भारत सरकार के मानव संसाधन विकास मंत्रालय द्वारा स्थापित एक स्वायतशासी संस्थान
INDIAN INSTITUTE OF SCIENCE EDUCATION & RESEARCH (IISER) - KOLKATA
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Established by the Ministry of Human Resource Development (MHRD), (An Autonomus Institution, Government of India).

Dr. Debasish Haldar, FRSC
Professor and HOD, Department of Chemical Sciences,
IISER Kolkata
Mohanpur, Nadia, West Bengal, India – 741246.

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IISER Kolkata, India, 16-01-2026

Message from the DCS Chairperson

I am delighted to know that the Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Kolkata is going to organize an International Conference entitled as "**Na**nomaterials and **Mo**lecules: From **S**pectroscopy to **Bio**imaging (**NaMoSBio 2026**)" during January 23-26, 2026.

This International Conference is intended to provide a suitable platform for cutting-edge research problems related to optical nanomaterials and molecules, their synthesis, single molecule/particle spectroscopy, ultrafast to slow exciton dynamics, theoretical/computational aspects, and applications like bioimaging, LEDs etc. and highlight recent advances. Internationally renowned researchers from different parts of the world will be presenting their top-notch research results in this conference. Graduate students from highly reputed Indian Institutes and Universities as well as our own Institute will be immensely benefited by interacting with the stalwarts in **NaMoSBio 2026**.

I wish this International Conference a great success.

Sincerely,

Debasish Haldar

Debasish Haldar
DCS Chairperson, IISER Kolkata

भारतीय विज्ञान शिक्षा और अनुसंधान संस्थान–कोलकाता
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INDIAN INSTITUTE OF SCIENCE EDUCATION & RESEARCH (IISER) - KOLKATA
Established by the Ministry of Human Resource Development (MHRD), (An Autonomus Institution, Government of India).
IISER KOLKATA

Dr. Prasun K. Mandal, Ph.D.
Professor, Department of Chemical Sciences,
IISER Kolkata, India.

Alexander von Humboldt Fellow
Marie Curie Fellow
Editorial Board Member, Scientific Reports (NPG)

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IISER Kolkata, India, 21-01-2026

Message from the Convenor

On behalf of the local organizing committee, it offers me immense pleasure to invite you to the International Conference entitled as "**Na**nomaterials and **Mo**lecules: From **S**pectroscopy to **Bio**imaging (**NaMoSBio 2026**)" at IISER Kolkata during January 23-26, 2026.

This conference will be attended by about 150 top-class and highly renowned researchers from different parts of the world. In this conference there will be 24 technical sessions, comprising of 5 Plenary Lectures, 12 Keynote Lectures, 23 Invited Lectures, 4 Short Talks and more interestingly, 5 young researchers will deliver the cutting-edge research of their early career in a special session called "Young-Investigators' Flash Presentation". Around 62 senior graduate students will present posters in the poster session on January 23 and 25, 2026.

This conference will not only provide a platform for intense discussions and fruitful interactions between top-class researchers at different stages of their career, but also promote collaborations between different groups from all over the world.

In this conference we will have a special prize for a good question asked during each and every lecture. I sincerely hope that the QnA session will be highly enjoyable in this conference.

Moreover, we are not specifically writing the role of the participants in this conference. Instead, the role of the participants can be understood in a subtle manner from the colour strip shown in their identity tag.

In this conference we will have a panel discussion with leading members from the government, industry and academia, regarding creating a synergy between government, institute and industry and I believe a constructive discussion will take place leading to a few key ideas that we can provide to the government, institutes and industry colleagues towards creating a synergy between these three pillars.

In spite of the busy conference schedule I believe the participants will have time to walk around the beautiful campus of IISER Kolkata. I hope that the participants will have an enjoyable stay at IISER Kolkata during this conference.

We are sincerely thankful to the sponsors of this conference. It would have been difficult to organize such a grand conference without their generous support.

Please enjoy this conference and feel free to contact me or the volunteers whenever necessary.

Sincerely,

Prasun K. Mandal

Prasun K. Mandal
Convener, **NaMoSBio 2026** International Conference
On behalf of the Organizing Committee of **NaMoSBio 2026** International Conference

About the Institute, IISER Kolkata:

Indian Institute of Science Education and Research Kolkata (IISER Kolkata) was established in 2006 by the Ministry of Human Resource Development (MHRD) (now Ministry of Education (MoE)), Government of India. IISER Kolkata is designed to reach the prestigious position in the global setting that IISc, IIMs and IITs presently enjoy. IISER Kolkata is an autonomous institution awarding its own degrees. The central theme of the IISER Kolkata is to integrate education with research so that undergraduate teaching as well as doctoral and postdoctoral research work could be carried out in basic sciences.

The basic idea of IISER is to create research Universities of the highest calibre in which teaching and education will be totally integrated with the state of the art research. These Universities are devoted to Undergraduate and Postgraduate teaching in sciences in an intellectually vibrant atmosphere of research. One of the important objectives of creating these Universities is to make education and careers in basic sciences more attractive by providing opportunities in integrative teaching and learning of sciences and break the barriers of traditional disciplines.

About the Department of Chemical Sciences, IISER Kolkata:

One of the first departments to be established in IISER Kolkata was the Department of Chemical Sciences (DCS). From the beginning, the Department has incarnated the Institute's mission of excellence in both research and teaching. The DCS has appreciable strength in the core areas of physical, organic and inorganic chemistry as well as in interdisciplinary research areas at the boundaries with physics, biology, earth science and materials science. An extremely wide range of state-of-the-art instrumentations are available in different research groups to carry out the DCS research activity.

The DCS researchers have made significant contributions in areas such as materials science, where they have developed new methods for the synthesis and characterization of functional materials for applications in energy storage and conversion. In self-healing crystals, the team has developed a novel method for creating crystal structures that can repair themselves in response to damage. In organic chemistry, the group has developed new reactions for the synthesis of complex organic molecules and explored the mechanisms of enzyme-catalyzed reactions. The DCS group has made significant contributions to all aspects of research in chemistry, including theoretical studies, synthetic methods, and materials design. These research efforts not only deepen our understanding of chemical science but also have the potential to contribute to numerous areas of societal significance, such as medicine, energy, and the environment.

NaMoSBio 2026: Schedule of the programme

Day 1: 23rd January 2026, Friday		
11.00-	Registration	
12:00-13:00	Inaugural Programme Welcome address by: • Prof. Debasish Haldar, Patron, NaMoSBio 2026 and DCS Chairperson, IISER Kolkata, India • Prof. Priyadarsi De, Dean, Research and Development, IISER Kolkata, India • Prof. D. D. Sarma, IISc, Bengaluru, India • Prof. Prasun K. Mandal, Convener, NaMoSBio 2026	
13:00-14:00	Pre-conference Lunch	
Session 1 Chair: Prof. Priyadarsi De, IISER Kolkata, India		
14:00-14:40	PL 1	*Title*: Everything You Wanted to Know About Mn Emission, But Were Afraid to Ask *Speaker:* Prof. D. D. Sarma, IISc, Bengaluru, India
14:40-15:10	KL 1	*Title*: DNA Nanotech for Brownian Computing and Molecular Robotics *Speaker:* Prof. Philip Tinnefeld, LMU München, Germany
15:10-15:30	IL 1	*Title*: Exploring Methods to Control The Emission Properties of Double Perovskites *Speaker:* Prof. Sameer Sapra, IIT Delhi, India
15:30-15:50	IL 2	*Title*: Visible-Light Photocatalysis with Quantum Dot-Sensitized Photon Upconversion *Speaker:* Prof. Pramod P. Pillai, IISER Pune, India
15:50-16:20	High Tea Break	
Session 2 Chair: Prof. Sayam Sen Gupta, IISER Kolkata, India		
16:20-16:50	KL 2	*Title*: Magneto-Plasmonics: Invoking Magnetic Response in Magnetic and Non-Magnetic Materials *Speaker:* Prof. Venu Gopal Achanta, CSIR-NPL, New Delhi, India
16:50-17:10	IL 3	*Title*: Teaching Molecules to Change Colour: Lessons from Chem 101 *Speaker:* Prof. Subhajit Bandyopadhyay, IISER Kolkata, India
17:10-17:25	ST 1	*Title*: Circularly Polarized Luminescent Nanomaterials and Assemblies: Exploring Optical Activity at The Nanoscale *Speaker:* Prof. Jatish Kumar, IISER Tirupati, India
17:25-17:35	YIFP 1	*Title*: Self-Trapped Excitons with Unusually Large Huang-Rhys Factor in Halide Double Perovskite Semiconductor $Cs_2AgInCl_6$ *Speaker*: Dr. Kingshuk Mukhuti, Radboud University, Netherlands
17:35-17:55	IL 4	*Title*: Controlling Photon Emission Statistics from Quantum Dots *Speaker:* Prof. Anshu Pandey, IISc, Bengaluru, India
Session 3 Chair: Prof. Raja Shunmugam, IISER Kolkata, India		
17:55-18:15	IL 5	*Title*: Water-Enhanced Deep Eutectic Electrolytes for Stable Zinc-Ion Batteries *Speaker*: Prof. Sayan Bagchi, CSIR-NCL Pune, India

18:15-18:35	IL 6	*Title*: Next Generation Dopants for Organic Electronics *Speaker*: Prof. Pabitra K. Nayak, TIFR Hyderabad, India
18:35-18:45	YIFP 2	*Title*: Non-Covalent Reversibly Photoswitchable Fluorescent Tags for Wash-Free Protein Labelling *Speaker:* Dr. Mrinal Mandal, ENS, Paris, France
Session 4 Chair: Prof. Ravi Kumar Kanaparthi, Central University of Kerala, India		
18:45-20:00	Poster Presentation (with Tea)	
20:00-22:00	Dinner	
Day 2: 24th January 2026, Saturday		
Session 5 Chair: Prof. Alakesh Bisai, IISER Kolkata, India		
09:00-09:40	PL 2	*Title*: First-Order Properties using The Relativistic Extended Coupled-Cluster Method *Speaker*: Prof. Sourav Pal, Ashoka University, India
09:40-10:10	KL 3	*Title*: Modeling Electrocatalysts for Hydrogen Evolution Reactions and Ultralow Lattice Thermal Conductivity in Topologically Non-Trivial $(Sb_2Te_3)_m(Sb_2)_n$ Homologous Series *Speaker*: Prof. Swapan K. Pati, JNCASR, Bengaluru, India
Session 6 Chair: Prof. Arabinda Chaudhuri, IISER Kolkata, India		
10:10-10:50	PL 3	*Title*: Exciton and Biexciton Dynamics in CdSe Nanoplatelets *Speaker*: Prof. K. George Thomas, IISER TVM, India
10:50-11:20	KL 4	*Title*: Functional Molecular Solids: Amorphous, Crystalline and Phase Change Materials, Structure-Phase Correlations *Speaker*: Prof. T. P. Radhakrishnan, University of Hyderabad, India
11:20-11:40	Tea Break	
Session 7 Chair: Prof. Kumaresh Ghosh, University of Kalyani, India		
11:40-12:00	IL 7	*Title*: Intracellular Subdegree Temperature Sensing and Dynamics by Thermoresponsive Silver Nanoclusters as Molecular Probes *Speaker*: Prof. Saptarshi Mukherjee, IISER Bhopal, India
12:00-12:20	IL 8	*Title*: Keeping The Chromophores Crossed for Efficient Photoinduced Symmetry-Breaking Charge Separation *Speaker*: Prof. Mahesh Hariharan, IISER TVM, India
Session 8 Chair: Prof. Tarun Kumar Mandal, IACS, Kolkata, India		
12:20-12:40	IL 9	*Title*: Tailoring Molecular Structure for Optimized Singlet Fission *Speaker*: Prof. Satish Patil, IISc, Bengaluru, India
12:40-13:00	IL 10	*Title*: Probing Singlet Exciton Fission in Molecular Cyclophane Dimers *Speaker*: Prof. Jyotishman Dasgupta, TIFR Mumbai, India
13:00-13:20	IL 11	*Title*: Electronic Structure and Mechanism of Singlet Fission *Speaker*: Prof. Debashree Ghosh, IACS, Kolkata, India

Session 9 Chair: Prof. Moloy Sarkar, NISER, Bhubaneswar, India		
13:20-13:30	Sponsor Talk 1	Gold Sponsor (ATOS)
13:30-13:35	Sponsor Talk 2	Bronze Sponsor (Scitech Incorporation)
13:35-14:30	Lunch Break	
Session 10 Chair: Prof. Soumyajit Roy, IISER Kolkata, India		
14:30-15:30	Panel Discussion	*Panellists*: • Prof. Thirumalachari Ramasami, Former Secretary, DST, India and Former Director, CLRI, Chennai, India • Dr. Samiran Mahapatra, R&D Director, Science & Technology, Unilever, India • Prof. Sourav Pal, Ashoka University, India and Former Director, IISER Kolkata, India • Prof. Venu Gopal Achanta, Director, CSIR-NPL, New Delhi, India • Prof. Anunay Samanta, University of Hyderabad, India • Prof. Priyadarsi De, Dean, Research and Development, IISER Kolkata, India
15:30-15:45	Group Photo Session	
15:45-16:00	High Tea Break	
16:00-	Bus leaves for Cruise Dinner on Ganges	
Day 3: 25th January 2026, Sunday		
Session 11 Chair: Prof. Mahesh Hariharan, IISER TVM, India		
09:00-09:40	PL 4	*Title*: Development and Characterization of Colloidal Nanoparticles Towards Applications in Life Science *Speaker*: Prof. Wolfgang Parak, University of Hamburg, Germany
09:40-10:10	KL 5	*Title*: Plasmonic Metal and Lead Halide Perovskite Nanocrystal Heterostructures *Speaker*: Prof. Narayan Pradhan, IACS, Kolkata, India
10:10-10:40	KL 6	*Title*: Perovskite Quantum Dots: From Minute to Femtosecond Spectroscopy *Speaker*: Prof. Quinten Akkerman, LMU München, Germany
10:40-11:00	Tea Break	
Session 12 Chair: Prof. Sanjib Bagchi, IISER Kolkata, India		
11:00-11:40	PL 5	*Title*: Charge Carrier Dynamics in Perovskite Nanocrystals *Speaker*: Prof. Anunay Samanta, University of Hyderabad, India
11:40-12:10	KL 7	*Title*: Defect-Mediated Electronic Processes in Perovskites Revealed by Luminescence: From Fundamentals to Neuromorphic Computing *Speaker*: Prof. Ivan G. Scheblykin, Lund University, Sweden

Session 13 Chair: Prof. T. P. Radhakrishnan, University of Hyderabad, India		
12:10-12:30	IL 12	*Title*: Visualizing Ribosomal-RNA Methylation Proteins in Action *Speaker*: Prof. Arindam Chowdhury, IIT Bombay, India
12:30-12:45	ST 2	*Title*: Enhancing Plasmonic Photocatalysis Through Ligand Engineering *Speaker*: Prof. Saumyakanti Khatua, IIT Gandhinagar, India
12:45-12:55	YIFP 3	*Title*: Interfacial Photophysics of Solar Cells with Non-Invasive Correlative Microscopy *Speaker*: Dr. Sudipta Seth, KU Leuven, Belgium
Session 14 Chair: Prof. Jatish Kumar, IISER Tirupati, India		
12:55-13:00	Sponsor Talk 3	Bronze Sponsor (Trokut Solutions)
13:00-13:05	Sponsor Talk 4	Bronze Sponsor (TCI Chemicals)
13:05-13:10	Sponsor Talk 5	Bronze Sponsor (Mono Scientific)
13:10-14:00	Lunch Break	
Session 15 Chair: Prof. Nikhil Guchhait, University of Calcutta, India		
14:00-14:30	KL 8	*Title*: Protein Structure, Drug Discovery, Diagnostics Using Light and Nanoparticles *Speaker*: Prof. Chandrabhas Narayana, JNCASR, Bengaluru, India
14:30-15:00	KL 9	*Title*: Harnessing Spin and Vibrations for Next Generation Molecular and Hybrid Optoelectronic Materials *Speaker*: Prof. Akshay Rao, University of Cambridge, UK
15:00-15:20	IL 13	*Title*: Polarization Engineering for Artificial Neural Circuits *Speaker*: Prof. Satyaprasad P Senanayak, NISER, Bhubaneswar, India
Session 16 Chair: Prof. Saptarshi Mukherjee, IISER Bhopal, India		
15:20-15:40	IL 14	*Title*: Vibronic Phosphorescence and Thermally Stimulated Delayed Phosphorescence: A Theoretical Perspective *Speaker:* Prof. Swapan Chakrabarti, University of Calcutta, India
15:40-16:00	IL 15	*Title*: Ionic Liquids in The Synthesis and Photophysical Modulation of Semiconductor Nanocrystals *Speaker:* Prof. Moloy Sarkar, NISER, Bhubaneswar, India
16:00-16:20	IL 16	*Title*: Fluorescent Materials: Self-Assembly and Photocatalytic Applications *Speaker*: Prof. Vandana Bhalla, Guru Nanak Dev University, Punjab, India
16:20-16:30	YIFP 4	*Title*: Decoupling Excitons from High-Frequency Vibrations in Organic Molecules *Speaker:* Dr. Pratyush Ghosh, University of Cambridge, UK
16:30-16:50	High Tea Break	

Session 17 Chair: Prof. Vandana Bhalla, Guru Nanak Dev University, Punjab, India		
16:50-17:20	KL 10	*Title*: Probing Carrier Relaxation Pathways in Lead- And Cadmium-Free Semiconductor Nanocrystals with Fast and Slow Spectroscopies *Speaker*: Prof. Łukasz Kłopotowski, Polish Academy of Sciences, Warsaw, Poland
17:20-17:40	IL 17	*Title*: What Drives Structural Distortions in Two Dimensional Hybrid Halide Perovskites? *Speaker*: Prof. Priya Mahadevan, SNBNCBS, Kolkata, India
17:40-17:55	ST 3	*Title*: Tuning Peptide Secondary Structure on Gold Nanoparticles Through Controlled Thiol and Carboxylate Functionalization *Speaker*: Prof. Anup Ghosh, Bose Institute, Kolkata, India
Session 18 Chair: Prof. Manoranjan Jana, University of Kalyani, India		
17:55-18:10	ST 4	*Title*: Exciton-to-Biexciton Transitions and Energy Transfer Dynamics in Mn-doped Perovskite Nanocrystals *Speaker:* Prof. Tushar Debnath, Shiv Nadar Institution of Eminence, Delhi, India
18:10-18:20	YIFP 5	*Title*: Tin vs. Lead Halide Perovskites: Interlinked Yet Distinct Colloidal Nanochemistries of Growth and Stability *Speaker:* Dr. Kushagra Gahlot, LMU München, Germany
Session 19 Chair: Prof. Saumyakanti Khatua, IIT Gandhinagar, India		
18:20-18:30	Sponsor Talk 6	Gold Sponsor (Laser Science)
18:30-18:35	Sponsor Talk 7	Silver Sponsor (Specialise Instruments)
18:35-18:40	Sponsor Talk 8	Bronze Sponsor (Horiba India)
Session 20 Chair: Prof. Aniruddha Paul, NIT Patna, India		
18:40-20:00	Poster Presentation (with Tea)	
20:00-22:00	Banquet Dinner	
Day 4: 26th January 2026, Monday		
Session 21 Chair: Prof. Amitava Das, IISER Kolkata, India		
09:00-09:30	KL 11	*Title*: Membrane Perturbations by Amphiphilic Molecules: A Worry and An Opportunity *Speaker*: Prof. Sudipta Maiti, BITS Pilani, Hyderabad Campus, India
09:30-09:50	IL 18	*Title*: Rashba and Excitonic Physics in Emerging Materials and Correlations with Light-Matter Interaction: A Computational Insight *Speaker*: Prof. Sudip Chakraborty, Harish-Chandra Research Institute, Prayagraj, India

Session 22 Chair: Prof. Pradip Kr. Ghorai, IISER Kolkata, India		
09:50-10:10	IL 19	*Title*: Conductivity in Battery Electrolyte Systems: Roles for Solution Structure, Ultrafast Solvent Modes and Ion-Ion Motional Correlations *Speaker*: Prof. Ranjit Biswas, SNBNCBS, Kolkata, India
10:10-10:30	IL 20	*Title*: Mapping Ultrafast Relaxation Dynamics of Large Stokes Shift Red Fluorescent Proteins *Speaker:* Prof. Arijit Kumar De, IISER Mohali, India
10:30-10:50	IL 21	*Title*: Halide Perovskite Nanomaterials for Energy and Optoelectronic Applications *Speaker:* Prof. Monojit Bag, IIT Roorkee, India
10:50-11:10	Tea Break	
Session 23 Chair: Prof. Balaram Mukhopadhyay, IISER Kolkata, India		
11:10-11:40	KL 12	*Title*: Chiral Metal Halide Crystals as Emerging Chiroptical Materials *Speaker*: Prof. Lakshminarayana Polavarapu, Universidade de Vigo, Vigo, Spain
11:40-12:00	IL 22	*Title*: Polymer Perovskite Composites for Energy Harvesting Applications *Speaker*: Prof. Aswani Yella, IIT Bombay, India
12:00-12:20	IL 23	*Title*: Developments in Cartesian-Grid-Based DFT in Atoms and Molecules (InDFT) *Speaker:* Prof. Amlan Kusum Roy, IISER Kolkata, India
Session 24 Chair: Prof. Ranjit Biswas, SNBNCBS, Kolkata, India		
12:20-12:45	Poster prize distribution	
12:45-13:00	Valedictory followed by vote of thanks	
13:00-	Lunch and Departure	

PL: Plenary Lecture

KL: Keynote Lecture

IL: Invited Lecture

ST: Short Talk

YIFP: Young Investigator’s Flash Presentation

Contents

Plenary Lectures

Everything You Wanted to Know about Mn Emission, But Were Afraid to Ask

D. D. Sarma

Solid State and Structural Chemistry (SSCU) Unit, Indian Institute of Science (IISc),
Bengaluru, Karnataka, India-560012.

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The highly efficient, sub-bandgap, orange emission from Mn^{2+} dopants in semiconductor quantum dot hosts has been the subject of over two thousand publications, owing to its broad scientific interest and technological potential. This emission, universally attributed to the $^4T_1 \rightarrow {}^6A_1$ transition of Mn^{2+}, is characterized by a long lifetime in the order of milliseconds and negligible self-absorption due to the large Stokes shift, holding promise for diverse applications.

Surprisingly, the fundamental aspect of how energy is transferred from the host to the Mn $^4T_1$ state, believed to occur extremely fast on the sub-ns scale, has not been understood so far.

In our work,[1,2] we investigate how the first excited multiplet state of Mn^{2+} ($^4T_1$) is populated from its $^6A_1$ ground state, which evidently requires spin-non-conserving processes, following photoabsorption in the host semiconductor nanocrystals. This seemingly simple question leads to several fundamental issues: What are the energy-transfer pathways from the host excited states to Mn^{2+}? How is the significant excess energy of the host excited state, compared to the energy of the Mn^{2+} $^4T_1$ state, defining the large Stokes shift, dissipated?

In this talk, I shall address critical gaps in our understanding of Mn emission from Mn-doped nanocrystal systems, using Mn@$CsPbCl_3$ as a generic platform. Through temperature-dependent steady-state and time-gated photoluminescence experiments, we demonstrate that the initial energy transfer proceeds to a highly excited Mn^{2+} multiplet under near-resonant conditions, rather than directly to the $^4T_1$ state. A cascade of spin-allowed transitions within the excited multiplet manifold, assisted by multiphonon processes, subsequently populates the $^4T_1$ state. This pathway explains both the pronounced low-temperature suppression of Mn^{2+} emission (due to a phonon bottleneck) and the universal scaling of dopant photoluminescence with respect to excitonic emission that we establish experimentally. We further develop and analytically solve rate equations that quantitatively and qualitatively account for all observations. We shall also demonstrate that the understanding of this system can be easily generalized to a large number of other systems, providing a basis for understanding dopant emissions in general.

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Bio-sketch

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First-Order Properties using The Relativistic Extended Coupled-Cluster Method

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Expectation value, Response approach, related Z-vector method, and stationary form of extended coupled cluster (ECC) method are well studied for first-order properties using the coupled-cluster method. Stationary methods have the potential of extension to higher order properties using (2n+1) rule. Seminal work has been done in the 80s and 90s from ours and other groups in the non-relativistic domain. In this talk, we will present the four-component relativistic approach using the ECC method for first-order properties, comparing with the other methods. We have calculated the P,T-odd sensitivity parameters of two moderately heavy laser-coolable diatomic molecules (SrH and SrF) in their ground electronic configuration state. The hyperfine structure (HFS) constants of Sr in the diatoms are also computed and compared with available experimental results to assess the accuracy of our calculations. The role of electron correlation, relativity, basis set and virtual spinors in ECC calculations are also investigated.

Keywords: Extended coupled-cluster method; Variational method; Relativistic effects; Z-vector technique; P,T-odd parameters

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Prof. Sourav Pal is currently a Professor and Head of the Department of Chemistry, at Ashoka University, India, and immediately before this was the Director of the Indian Institute of Science Education and Research (IISER) Kolkata from October 2017 to October 2022. Before joining IISER Kolkata he was a professor at the Indian Institute of Technology Bombay from May 2015. Before joining IITB, he was also the Director of CSIR-National Chemical Laboratory (NCL), Pune for five years and was an eminent scientist at NCL Pune for almost 33 years. He was instrumental in establishing a core theoretical research group, the Electronic Structure Theory Group at NCL. He is a distinguished theoretical chemist and has contributed to methodological and conceptual developments on many-body electronic structure theory, to the area of density-based chemical reactivity as well as to catalytic and hydrogen storage materials using computational material science. He has made outstanding contributions to the development of rigorous *ab initio* theory for molecular electronic structure and the various aspects of multireference coupled cluster approach to molecular properties including spectra and other allied areas. He was honored by delivering the Charles A. Coulson lecture at the University of Georgia in 2014.

Degrees and Honour appointments:

He obtained his 5 years integrated Master's degree in Chemistry from the Indian Institute of Technology (IIT) Kanpur in 1977, received a Ph.D. degree from Calcutta University, and joined NCL in 1982 as a scientist. He was a post-doctoral fellow at the University of Florida, Gainesville, USA (1986-87) and has been an Alexander von Humboldt Fellow at the University of Heidelberg, Germany (1987). He has been a visiting Professor at the University of Arizona, Tucson, USA, the University of Torun, Poland, and the Institute for Molecular Sciences, Okazaki, Japan. He also holds an Adjunct Professorship at IISER Pune and IIT Goa.

Membership of committee and Science Administration:

Prof Pal has served as an academic administrator very effectively along with a distinguished research career. He served as the President of the Chemical Research Society of India for three years from 2014-2017. **He was a member of the Executive Council of the Federation of Asian Chemical Societies and also served as a member of the founding Executive Board of the Commonwealth Chemical Sciences for three years (2020-23).** As a member of the Executive Board, he played a key role in pushing the Commonwealth vision of gender equality, Sustainable development goals, and access across the Commonwealth nations. He is currently a member of the Finance Committee of the Commonwealth Chemistry. **He is elected as a Member of the Board of the Asia-Pacific Association of Theoretical and Computational Chemists (APATCC) and a Member of the Science Education Committee under the Association of Academies and Societies of Sciences in Asia (AASSA).** He is also a member of the National Advisory Board of the International Society of Theoretical Chemical Physics (ISTCP).

In addition, he has served on several important scientific committees/bodies in India. **He is presently the Chairman of the Chemical Division Council of the Bureau of Indian Standards (BIS), an important position in BIS setting standards of industries in India.** He has been continuing in this coveted position since 2014. He was a member of the Council of the Indian National Science Academy, New Delhi. **He has also contributed to several outreach activities through CRSI, ACS, and RSC. He was Chairman of the Western India RSC Chapter for three years from 2011 to 2014 and remained associated with RSC India. He has also conducted an NPTEL course on Many-body methods in chemistry and a NPTEL+ workshop on computational chemistry and DFT in last one year.**

Awards and Honours (Selected list):

He has been recognized with several prominent awards and honors for his contributions to science, including the prestigious Shanti Swarup Bhatnagar Award in Chemical Sciences in 2000 and the first SASTRA-CNR Rao Award in Chemistry & Materials Science for the year 2014 and many others. He is a Fellow of the Royal Society of Chemistry, 2011, the Indian National Science Academy (2003), the Indian Academy of Sciences (1996), and National Academy of Sciences (1998), the Royal Society of Chemistry (2011), and the Maharashtra Academy of Sciences (1994). He has been the J C Bose National Fellow of the Department of Science and Technology since 2008. He has been honoured with Lifetime achievement award of Chirantan Rasayan Sanstha (CRS).

He was on the Editorial Advisory Board of the Journal of Physical Chemistry, **has guided more than 45 Ph.D. theses, and has published about 320 research papers in international peer-reviewed journals.** He has authored a book titled "Mathematics in Chemistry" and contributed to chapters in several books. He has recently co-edited an e book (Springer Nature) on 'Development of Theoretical Methods, Algorithms and Applications' . He has organized many key conferences. He has been invited to deliver plenary/keynote/highlighted lectures in several institutions and international conferences of repute over the years in India and abroad. Very recently he delivered a keynote talk at QSCP27 at Paris.

Exciton and Biexciton Dynamics in CdSe Nanoplatelets

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Developing semiconductor systems for light-energy harvesting and optoelectronic applications requires a detailed understanding of exciton and biexciton dynamics, as well as charge delocalization of photogenerated carriers.[1-4] The first part of the presentation will discuss the effect of excitation energy on biexciton dynamics in CdSe-based nanoplatelets (NPLs), investigated using ensemble and time-resolved single-particle spectroscopy. By varying the excitation energy from 3.1 eV to 2.1 eV, the biexciton-to-single-exciton quantum yield increases from 36% to 75%. These results indicate that the non-radiative Auger recombination process is largely independent of the excitation energy. In the second part, I will describe the influence of plasmonic fields on the photoluminescence (PL) properties of CdSe NPLs coupled to Au nanofilms, achieved by precisely controlling the separation distance between the two components. I will further discuss how plasmonic coupling modifies PL lifetimes associated with first- and second-exciton recombination in a cascade two-photon emission process. The third part of the presentation focuses on the impact of Ag^+ ion doping on the PL dynamics of CdSe NPLs. In addition to the sharp band-edge emission of CdSe NPLs, doping with 1 atom% Ag^+ introduces a broad, red-shifted emission. The observed anticorrelated switching between the band-edge and dopant-mediated emission channels suggests a dynamic exchange between these two recombination pathways.

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Bio-sketch

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K. George Thomas is a Senior Professor at the School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram (www.kgtlab.in), and has made significant contributions to photosciences and nanomaterials. His current research focuses on light–matter interactions at the nanoscale. He received his Ph.D. in Chemistry from the University of Kerala and served as a Senior Scientist at the CSIR–National Institute for Interdisciplinary Science & Technology from 1994 to 2010, before joining IISER Thiruvananthapuram as a Professor in 2010, following an invitation. He has published ~140 peer-reviewed research articles (h-index 52, average citation per article ~100) and has mentored 33 Ph.D. scholars, many of them holding faculty positions in leading institutions in India and abroad. He is a recipient of several awards and distinctions, including the Shanti Swarup Bhatnagar Prize in Chemical Sciences (2006) and the J. C. Bose National Fellowship (2014–2024). He is an elected Fellow of the Indian Academy of Sciences (2007) and the Indian National Science Academy (2015).

Development and Characterization of Colloidal Nanoparticles Towards Applications in Life Science

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Materials development and characterization of colloidal nanoparticles towards applications in life science. For solving scientific questions in life sciences it is helpful having a large variety of toolkits and assays. Materials science can contribute in this direction by synthesis of new materials and analysis techniques. Nanomaterials together with synchroton radiation are an example in this direction which could be helpful towards developing future nanomedicines. These techniques can be for example applied to fate mapping and degradation studies.

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Bio-sketch

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Wolfgang Parak is Professor at the University of Hamburg. He has studied physics and obtained his PhD in Munich. After a postdoctoral fellowship at Berkeley he returned 2003 to Munich to start his own group. Before moving to the University of Hamburg in 2017 he spent 10 years as professor at the Philipps University Marburg. The research of Wolfgang Parak is dedicated towards the development of new surface chemistries of inorganic nanoparticles and towards the characterization of their physicochemical properties. In particular, the development of an amphiphilic polymer coating is nowadays used by many different groups worldwide. Nanoparticles with such high colloidal stability are the bases of experimentally correlating their physicochemical properties with their interaction will cells (involving uptake and cytotoxicity), which has been the research topic of the Parak group for the 2 decades. The group also uses polymeric polyelectrolyte capsules fabricated by layer-by-layer assembly for biological applications (in vitro sensing and delivery).

Charge Carrier Dynamics in Perovskite Nanocrystals

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The lead halide-based hybrid and all-inorganic perovskites are currently the focus of intense investigation because of their potential in solar photovoltaic and light-emitting applications.[1] Considering the fact that our understanding of the fundamental photo-processes in these systems like the deactivation pathways and dynamics of the photo-generated charge carriers, which is essential for proper utilization of these substances in different applications, is still limited, we have been looking into these substances addressing a variety of issues including those mentioned above. This talk will focus on how a combination of femtosecond pump-probe and single-particle fluorescence techniques can provide valuable information on the nature and energy states of the photogenerated species, pathways and dynamics of relaxation of the charge carriers, location and nature of the trap states and their role in fluctuation of the photoluminescence of different caesium lead halide ($CsPbX_3$) perovskite nanocrystals.[2-5]

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Bio-sketch

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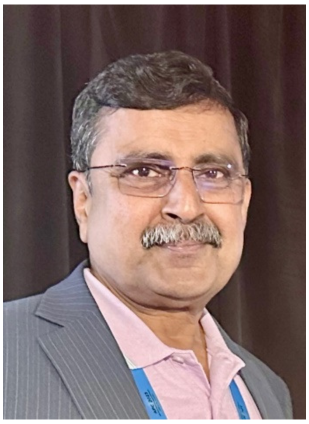

Anunay Samanta is currently INSA Senior Scientist and Emeritus Professor at the University of Hyderabad. He has been at this place since 1990 after obtaining Ph.D. (1987) from Indian Association for the Cultivation of Science (Jadavpur University), Kolkata and spending a couple of years at the Radiation Laboratory, University of Notre Dame, USA as a postdoctoral fellow. His current research focuses on probing charge carrier dynamics in perovskite nanocrystals employing ultrafast pump-probe and single-molecule photoluminescence techniques. interest lies in ultrafast dynamics and single-molecule spectroscopy of the perovskite nanocrystals. He is a Fellow of the Science Academies of India and recipient of many national and international awards, which include the J.C. Bose National Fellowship, Thomson Reuters India Citation Award, Raman-Mizushima Lecture Award, APA Award, Masuhara Lectureship Award and Visitor’s Award.

Keynote Lectures

DNA Nanotech for Brownian Computing and Molecular Robotics

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Merging DNA nanotech with single-molecule detection allows visualizing molecular processes with ultimate resolution and sensitivity. Here, we show how DNA origami can be the key to advance biosensing schemes with respect to sensitivity, specificity and programmability. Fluorescence signals are physically enhanced by DNA origami nanoantennas for attomolar detection of pathogenic nucleic acids towards points of care molecular diagnostics.[1,2] Biosensors are adapted in the working range and cooperativity without changing the biorecognition elements using avidity and lever effects.[3] Combining different dynamic DNA elements allows DNA computing that benefits from Brownian motion and does not protect the stability of states against it. The vision is to develop molecular robotic systems that process complex inputs, compute autonomously, and provide light signals or cargo release as output.[4,5]

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Philip Tinnefeld is director of the chemistry department and chair of physical chemistry at LMU Munich. He leads an interdisciplinary research group in single-molecule spectroscopy, super-resolution microscopy, DNA nanotechnology and biosensing with a focus on method development. He has contributed to breakthroughs in super-resolution microscopy with the techniques dSTORM, DNA-PAINT and pMINFLUX. Recently, he combined single-molecule detection with DNA nanotechnology to develop self-assembled functional devices, biosensors and nano-robots. In addition to more than 200 peer-reviewed publications, he is involved in 10 patent applications and is initiator of GATTAquant, the first company for DNA origami applications.

Magneto-Plasmonics: Invoking Magnetic Response in Magnetic and Non-Magnetic Materials

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Magneto-optical responses are generally weak and require enhancement for more device applications. Plasmon-mediated enhancement of magneto-optical properties showed orders of magnitude improvement in Faraday and Kerr effects. In addition to the magneto-plasmonic crystals, quasi-periodic structures based on metal-dielectric nanopatterns have been demonstrated for broadband response. For functional or active devices that can be controlled by application of external magnetic or electrical fields, invoking electromagnetic responses would be very interesting. This is especially true if one can invoke functionality in existing electronic or optoelectronic devices by a simple modification to the existing device architecture.

Magneto-optical effects are governed by the off-diagonal elements of the dielectric tensor and are manifestations of time reversal symmetry breaking. For given naturally existing materials, the magneto-optical response is fixed based on the dielectric tensor. These values are, typically, weak and limits the device applicability. Magneto-plasmonic crystals are metal-dielectric nanostructures with periodic patterns in which magneto-optical properties are enhanced through plasmon mediation. Upto 3 orders of magnitude of enhancement as well as novel effects are demonstrated.

In this talk, after introducing magneto-plasmonics, I will present novel nanophotonic structures in which magnetic response can be invoked even in non-magnetic materials.

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Prof. Venu Gopal Achanta obtained his Ph.D. (Physics) from TIFR, Mumbai and Ph.D. (Electronics) from Tokyo University. He is currently the Director of CSIR-National Physical Laboratory. He is on lien from Tata Institute of Fundamental Research, Mumbai where he is a Professor. His research interests are in the application of nanophotonics to single molecule and single photon spectroscopy through light-matter interaction in non-perturbative regimes. He has over 150 journal publications. He is a Fellow of the Optica - Optical Society of America, and the Indian National Science Academy (INSA) and an honorary fellow of the Metrology Society of India (MSI). He is elected to the International Committee for Weights and Measures (CIPM) in 2022, to the Commission C2 of IUPAP in 2024, and to the executive committee of Asia Pacific Metrology Program (APMP). He is currently President of Optical Society of India (OSI), and Vice president of Indian Laser Association (ILA), and is on the EC of IEEE Photonics Mumbai Chapter. He is a member of the Empowered Board of LIGO, India, and senate member of IIT, Delhi and JNU, New Delhi.

Modeling Electrocatalysts for Hydrogen Evolution Reactions and Ultralow Lattice Thermal Conductivity in Topologically Non-Trivial $(Sb_2Te_3)_m(Sb_2)_n$ Homologous Series

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In this talk, I shall discuss our efforts on modeling single atom fullerene electrocatalysts for splitting water for generating hydrogen and oxygen evolution reactions (OER).[1] We have studied photocatalytic and electrocatalytic hydrogen evolution reaction in tetrazine-based covalent organic framework.[2] Furthermore, I shall discuss the effect of hydrostatic pressure and external strain on the topologically non-trivial $(Sb_2Te_3)_m(Sb_2)_n$ homologous series. While they show low thermal conductivity for topological reasons, we also have studied their phase transition on when external pressure and strain are applied to some of the topologically insulating materials.[3]

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Bio-sketch

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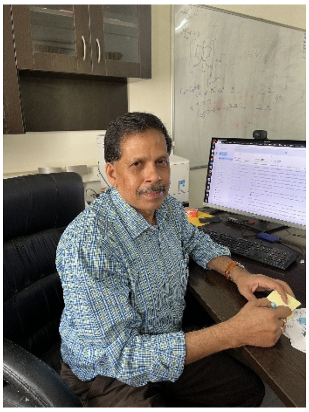

Professor Swapan K. Pati obtained his PhD from Indian Institute of Science, Bangalore followed by postdoctoral work at University of California, Davis, and Northwestern University, USA. He joined Theoretical Sciences Unit in JNCASR in November 2000 as an Assistant Professor and in June 2009, he became the full Professor. He has received MRSI (2006), CRSI bronze (2007) and BM Birla medals (2008); Swarnajayanthi Fellowship (2007-12), S. S. Bhatnagar award (2010) and The World Academy of Sciences award (2012). He is a recipient of J. C. Bose national fellowship in 2013, in 2018 and in 2023. He is an elected fellow of IASc (2009), NASI (2010), TWAS (2015) and INSA (2018). His research interests include designing materials for microscopic understanding and for application purposes. Some of the current projects in the lab include, modelling (i) catalytic processes for energy, (ii) Finding quantum spin liquid phase in (non) frustrated magnetic materials (iii) materials for anode/cathode for metal ion battery, (iii) generalized transport phenomena, including heat to current (thermoelectric), light to voltage (photovoltaics) and advanced transistor (FET) devices, (iv) phase transitions and new and exotic phases in dipolar Bosonic and Fermionic optical lattice systems. He is also involved in developing new theoretical tools for studying non-equilibrium phenomena.

Functional Molecular Solids: Amorphous, Crystalline and Phase Change Materials, Structure-Phase Correlations

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Evolution of functional molecular materials has followed established phenomena in the traditional solid state, but with fundamentally new paradigms;[1] novel frontiers continue to emerge. The assembly and attributes of molecular materials can be tuned by subtly modulating the non-covalent intermolecular interactions. Basic exploration of the crystalline (**C**) / amorphous (**A**) assemblies of these materials raise fundamental questions. The strongly zwitterionic diaminodicyanoquinodimethane (DADQ) based molecules exhibit not only appreciable NLO responses,[1] but also enhanced fluorescence in the aggregated/solid states. We have shown that the oriented aggregation of the molecules play a critical role,[2] and that the crystallinity is a tuneable parameter in their hierarchical assembly.[3] Bio-imaging,[4] electron beam triggered actuation,[5] and dielectric tuning of the emission[6] were also demonstrated in these materials. DADQs provide a facile platform to explore the **A**→**C** transformation in nanoparticles,[7] and thermally-induced reversible **A**⇌**C** transitions accompanied by prominent fluorescence switching;[8] the latter marked the entry into a new domain of functional molecular phase change materials (PCMs), and enabled direct laser write-read-erase in nanocomposite thin films.[9] We will present these aspects of functional molecular PCMs, and close with a discussion of the basic insights into the molecular structural control of the **A**-**C** balance in solids through a novel structure-phase correlation developed using the DADQs.[10]

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Bio-sketch

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Plasmonic Metal and Lead Halide Perovskite Nanocrystal Heterostructures

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Metal-semiconductor nanocrystal heterostructures have been extensively studied for decades for their efficient light harvesting and charge-transfer properties. Heterostructures of gold and silver nanoparticles with chalcogenides are the most widely studied. The photophysical properties and the plasmon induced change in the recombination process are the most important optical features of these nanocrystals and moreover the generated charge carriers efficiently move because of the plasmon-exciton coupling. However, for halide perovskites such heterostructures could not have been established yet and hence, the plasmon induced change in the photophysical processed could not be studied. In this presentation, the chemistry of epitaxial heterostructures of Au-$CsPbBr_3$ nanocrystals will be presented and the heteronucleations of Au on the halide perovskite semiconductor and the epitaxial relations will be extensively discussed. Using HRSTEM imaging, the inter-plane interactions of these cubic-orthorhombic phase of two nanostructures have been analysed and the change in optical properties in such structures are established. The same for Ag-CsPbBr3 will also be presented. In addition, other non-plasmonic heterostructures with halide perovskites will also be discussed.

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Narayan Pradhan works on semiconductor nanocrystals and currently he is a senior professor in the school of materials sciences at Indian Association for the cultivation of sciences, Kolkata.

Perovskite Quantum Dots: From Minute to Femtosecond Spectroscopy

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Colloidal lead halide perovskites (LHP) nanocrystals (NCs) are popular light-emissive materials for optoelectronic devices, of interest for LEDs, LCDs, lasers and quantum light sources. Most studies on LHP NCs focus on relatively large NCs exceeding 10 nm in size, exhibiting weak to no quantum confinement effects. Recently, we showed that perovskite quantum dots (pQDs) can be synthesized using a newly developed synthesis route, resulting in pQDs that are tunable between 3 and 13 nm range.[1]

Spectroscopy has always played a key role in understanding both the chemical and physical properties of quantum dots, as is also the case for perovskite QDs. Particularly, the soft and ionic nature of perovskites strongly influences many properties. In this talk, I will discuss how we use both in situ spectroscopy and transient absorption spectroscopy ranging from measurements on the minute scales all the way to the femtosecond time scales. This includes the growth and nucleation of the pQDs,[1] their ionic halide exchanges,[2] excitons in these QDs,[3] exciton-exciton interactions,[4] as well as exciton phonon interactions. This highlights the many unique structure and optical properties of pQDs.

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Bio-sketch

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Career History:

–2021 – present: **Research team Leader**, LMU München, D
–2020 – 2021: **Postdoctoral Researcher**, ETH Zürich, CH
–2014 – 2019: **PhD Degree**, Istituto Italiano di Tecnologia (IIT), Genova, IT
–2008 – 2014: **Bacholor** and **Master degree**, University of Utrecht, Utrecht, NL

Summary:

Quinten Akkerman earned his PhD in (2019) at Istituto Italiano di Tecnologia in Genova, Italy. After this, he was postdoctoral researcher at ETH Zürich (Switzerland, 2020-2021) and he is currently a group leader at the LMU München (Germany, 2021-present). His work is focused on the synthesis and optical properties of solution-grown nanocrystals, with a current focus on perovskite quantum dots. The quality of his research is confirmed by over 50 publications in high-impact factor journals, including: Science, Nature Materials, Nature Energy, Materials Today, ACS Energy Letters, Journal of the American Chemical Society. Quinten has an h-index of 36 and over 12.000 citations.

Awards/Grants:

2025 – ERC Starting Grant

Defect-Mediated Electronic Processes in Perovskites Revealed by Luminescence: From Fundamentals to Neuromorphic Computing

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Methods inspired by single-molecule spectroscopy, traditionally applied to molecules and quantum dots, have proven highly effective for investigating sub-micrometer metal-halide perovskite crystals and thin films. In these nano-structured systems, charge dynamics are often governed by only a few discrete carriers and defect states, leading to a so-called “digitized” regimes where conventional continuous semiconductor models no longer directly apply.[1] Phenomena such as blinking photoluminescence expose metastable non-radiative centers, effects of ion migration and self-healing.[2] We further demonstrate that crystal size beyond the quantum confinement effect plays an important role in determining the photoluminescence quantum yield (PLQY), underscoring the importance of spatial structure in the range 50 - 200 nm in luminescent materials.

Furthermore, we explore how charge trapping induces memory effects in the PL response, forming the basis for an optical memristor, or memlumor—a luminescent memory element with state-dependent PLQY.[3] These perovskite-based memlumors leverage photodoping and photochemistry to encode volatile and non-volatile optical memory over timescales from nanoseconds to days. Using a novel multi-pulse time-resolved PL technique, we demonstrate ultralow switching energies (in the femtojoule range) and sub-microsecond classification of binary optical pulse patterns, positioning memlumors as promising components for neuromorphic optical computing.[4]

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Bio-sketch

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Ivan Scheblykin received his Ph.D. in 1999 from the Moscow Institute of Physics and Technology and the Lebedev Physical Institute of the Russian Academy of Sciences, where he studied exciton dynamics in J-aggregates. After a postdoctoral fellowship at KU Leuven, Belgium, he moved to Sweden in 2002 to establish the Single Molecule Spectroscopy Group at Lund University's Division of Chemical Physics, becoming a full professor in 2014. His research focuses on the fundamental photophysics of organic and inorganic semiconductors, with emphasis on energy transfer, charge migration, and trapping. A central theme of his work is uncovering physical and chemical processes that lie beyond ensemble averaging in optoelectronic materials, with current interests in charge dynamics in perovskite semiconductors. He is widely recognized for his expertise in photoluminescence spectroscopy, including time-resolved and single-molecule techniques.

Protein Structure, Drug Discovery, Diagnostics Using Light and Nanoparticles

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The talk is going to dwell in the realms of discovering the therapeutically important protein structure using Raman spectroscopy and molecular dynamics simulations using noble metal nanoparticles. Xray crystallography of protein crystals is the golden standard for determining the structure of proteins, and recently the cryo-EM has made it easy to determine the structures. Even with large developments in this field there are many proteins where structures are difficult to determine. We in our group has worked with such proteins or proteins where the structures exist to understand the protein structure function in their physiological conditions. We have been able to use this to do drug screening and diagnostics. The talk will elucidate this with various examples from our group.

Bio-sketch

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Prof. Chandrabhas Narayana obtained his Ph.D. from the Indian Institute of Science, Bangalore in 1995 and carried out postdoctoral research in the Materials Science and Engineering Department of Cornell University, New York from 1995 to 1998. He joined JNCASR as an Assistant Professor in 1998. He is Professor at Chemistry and Physics of Materials Unit of JNCASR. He has been the Dean, Fellowships and Extension Programs, and Dean, Research and Development at JNCASR. He also was the Chairman of Chemistry and Physics of Materials. He was the Director of Rajiv Gandhi Centre for Biotechnology, Thiruvananthapuram, Kerala for past 5 years. He works in the areas of Condensed Matter Physics, Chemistry, Nanomaterials, Material Science and Biology. He is an expert in the use of Raman spectroscopy, high pressure, X-ray diffraction and uses these to understand the physical properties of materials.

Awards, Honors, & Fellowships:

- Fellow of the Kerala Academy of Sciences, 2023
- Fellow of the Indian Society of Analytical Scientists, 2022
- Fellow, Indian Academy of Sciences (FASc), 2018
- Fellow, Royal Society of Chemistry (FRSC), 2017
- Fellow, India National Academy of Sciences (FNASc), 2012

- A P J Abdul Kalam National Award, 2024
- Sir C. V. Raman Memorial Award Lecture of the Indian Photobiology Society
- Dr. Taranath Shetty Memorial Oration Award Popular Lecture Series of Association of Clinical Biochemists of India, 2023
- ISAS Raja Ramanna Award, 2022
- Platinum Jubilee Lecture Award of the Indian Science Congress, 2020
- Mizushima Raman Lecture Award, 2018
- MRSI-ICSC Superconductivity & Materials Science Senior Award, 2017
- Sir C.V. Raman Young Scientist Award (Karnataka Government), 2008
- Bronze Medal, Material Research Society of India, 2007

Harnessing Spin and Vibrations for Next Generation Molecular and Hybrid Optoelectronic Materials

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For fifty years, the design of π-conjugated organic materials, the cornerstone of technologies from organic light emitting diodes (OLEDs) to fluorescent markers that have brought revolutionary advances in bio-imaging, DNA sequencing and medical diagnostics, has been governed by a central challenge: mitigating the detrimental effects of spin-1 triplet excitons and strong exciton-vibrational coupling. These phenomena are responsible for fundamental limitations such as homogeneous line broadening, with emission linewidths often exceeding 300 meV; fast non-radiative decay that severely limits photoluminescence quantum efficiency (PLQE) of near-IR (NIR) emission and the performance of organic photovoltaics (OPVs); self-trapping and scattering of excitons leading to slow FRET based transport. Current state-of-the-art strategies, such as phosphorescent materials or thermally activated delayed fluorescence (TADF) materials, are ultimately workarounds that accept these properties as unavoidable constraints.

Recent breakthroughs from my group suggest a path to overturn this decades-old paradigm. In this talk I will share some of this recent work and discuss how it could help us move from mitigating limitations to actively harnessing spin and vibrations, establishing new physical insights and new design rules for molecular and hybrid systems to unlock materials and device performance far beyond the current state of the art, thereby enabling transformative technologies.

Bio-sketch

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Akshay is Professor of Physics at the Cavendish Laboratory, University of Cambridge. He obtained in BSc from St Stephen's College, University of Delhi, in 2006 and MSc from the University of Sheffield in 2007. He completed his Ph.D. from the University of Cambridge in 2011 under the supervision of Prof. Sir Richard Friend, following which he held a Junior Research Fellowship (JRF) at Corpus Christi College, before establishing his independent research group in 2014.

His research interests lie in the study energy and nanoscale materials, in particular to elucidate the fundamental electronic, structural and transport dynamics of these materials and help guide the design of new materials and devices for applications in photovoltaics, LEDs and batteries. He has pioneered a new generation of optical spectroscopy and microscopy experiments that are allowing us to understand these materials with unprecedented spatial and temporal precision. He was awarded the Institute of Physics Henry Morsely Medal and Prize for "Outstanding early-career contributions to Physics".

He is co-founder of Cambridge Photon Technology (https://www.cambridgephoton.com/) and illumion (https://www.illumion.io).

CPT was founded in January 2020 and is engaged in the commercialisation of a new quantum photonics technology that Akshay invented, the "Singlet Fission Photon-Multiplier", which has the potential to break the single-junction efficiency limit (Shockley–Queisser limit) which holds back all single junction photovoltaics. If successful, this could add 10% to the efficiency of Si based photovoltaics. CPT has raised significant funding and is working with a range of industrial partners including some of the largest Si PV manufacturers. CPT has won the Royal Society of Chemistry Emerging Technologies Prize, has been named a Deep Tech Pioneer and was a Regional Prize winner of Shell's Springboard Competition for the UK's most promising new low-carbon enterprises.

illumion was founded in 2022, to commercialising Charge Photometry, a new optics methodology invited by Akshay. Charge photometry is a light scattering microscopy technique that visualizes state-of-charge changes in individual active particles during battery cycling. It exploits the principles of optical interference reflection microscopy to detect scattered light from the active particles. Ion insertion and extraction in the active particles give rise to changes in the detected optical contrast, reporting on the local state-of-charge. We envision that this platform could become an indispensable part of battery research both in industry and academia, helping to accelerate the development of new battery technologies.

Probing Carrier Relaxation Pathways in Lead- And Cadmium-Free Semiconductor Nanocrystals with Fast and Slow Spectroscopies

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Semiconductor nanocrystals have garnered the attention of chemists, physicists, and engineers as versatile materials with unique properties and exciting potential applications. The best known compounds are lead and cadmium chalcogenides and lead halide perovskites. However, the concerns related to toxicity of lead and cadmium ions have inspired a quest to find alternatives. In this talk, I will present our work on multinary nanocrystals based on I-III-VI compounds and on double perovskites. In particular, I will talk about our efforts to understand the mechanism of light emission by these nanostructures. I will discuss the results of temperature and magnetic field dependent photoluminescence dynamics, room temperature transient absorption, and single nanocrystal spectroscopy.

Bio-sketch

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I lead a research group at the Institute of Physics, Polish Academy of Sciences in Warsaw, Poland. In our research, we focus on novel, exciting, and application-relevant colloidal nanomaterials. We mainly work with lead- and cadmium-free compounds, but we do detours into (the irresistible) lead halide perovskites. We apply advanced spectroscopic tools to obtain a state-of-the-art understanding of carrier relaxation pathways and properties of light emission from the studied nanostructures. In particular, we employ high throughput single particle spectroscopy to study the emission properties at the single nanostructure level and to generalize the conclusions to whole ensembles.

Membrane Perturbations by Amphiphilic Molecules: A Worry and An Opportunity

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The lipid membrane directly or indirectly controls many cellular functions. Small amphiphilic molecules and lipids such as cholesterol easily perturb membrane properties. Here we probe how such perturbations modulate cellular functions. We develop quantitative assays for probing how small amphiphiles modulate the properties of artificial bilayers and show that these assays correlate remarkably well with how these amphiphiles affect exocytosis in living cells. Using these tools, we find that monoamines (serotonin and its chemical analogues) modulate membrane properties in a manner that promotes exocytosis in cultured neurons. In contrast, the reduction of cholesterol changes membrane properties in the opposite manner and inhibits exocytosis. This is a potential collateral effect of chronic use of cholesterol-lowering drugs such as statins. In addition, we explore psychedelic substances (such as DOI) that have been found to promote neuronal plasticity and ask whether these effects may correlate with their ability to perturb the membrane. We find that DOI can cause very strong membrane perturbations, which can in principle affect cellular processes. Our findings highlight the possibility of designing novel membrane-targeting drugs, especially for controlling neuronal processes.

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Sudipta Maiti is a Senior Professor with joint appointment in the Departments of Biological Sciences and Physics in the Hyderabad campus of the Birla Institute of Technology and Science Pilani, India. Till 2024, he was Senior Professor and Chair of the Dept. of Chemical Sciences at the Tata Institute of Fundamental Research, Mumbai, India. He has an undergraduate degree in Physics from IIT Kanpur and a Ph.D. in ultrafast spectroscopy from the Univ. of Pennsylvania. Subsequently, he was a post-doctoral fellow in the lab of Prof. Watt Webb at Cornell university. His current research interest spans several areas of Biophysics, namely, protein aggregation, neurotransmission, membrane interactions, and the development of new techniques and instruments for studying biological phenomena (see biophotonics.co.in). He has built, patented and commercialized high-end microscopy and spectroscopy instruments. He is also a passionate community builder and teacher. He co-founded the Fluorescence Society (fluorescenceindia.org) and initiated an annual national workshop to teach graduate students how to build optical tools. He is currently the President of the International Society on Optics Within Life Sciences (Germany, owls-society.org), past-president of the Indian Biophysical Society, and the Chair-Elect of the Fluorescence Subgroup, Biophysical Society (USA). He is a Fellow of the Indian Academy of Sciences and an Executive Editor of the Journal of Physical Chemistry of the American Chemical Society.

Chiral Metal Halide Crystals as Emerging Chiroptical Materials

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Over the last decade, metal halide perovskite nanocrystals (LHP NCs) and their derivatives, in the form of nano and bulk crystals, have emerged as a promising class of semiconductor materials with many interesting linear and nonlinear optical properties. The light emission of LHP NCs is not only tunable by their dimensions and composition but also through self-assembly into ordered architectures. Interestingly, LHP NCs spontaneously self-assemble into superlattices and exhibit interesting optical properties such as polarized emission. On the other hand, low-dimensional metal halide crystals with chiral ligands exhibit chiroptical properties. This talk will be focused on the latest developments in achieving polarized absorption and emission from metal halide bulk and nanocrystals either by self-assembly of NCs or helical structural engineering.

Bio-sketch

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Lakshminarayana Polavarapu is the principal investigator of the Materials Chemistry and Physics research group at the Centro De Investigaciones Biomédicas (CINBIO), and associate professor in the department of physical chemistry at the University of Vigo. He obtained an M.Sc. in chemistry from the University of Hyderabad (India) and a Ph.D. from the National University of Singapore. After being a postdoctoral fellow at CIC biomaGUNE and the University of Vigo in Spain, he joined the Chair for Photonics and Optoelectronics at the Ludwig-Maximilians-University of Munich (Germany) as an Alexander von Humboldt postdoctoral fellow. He later continued as a junior group leader until May 2020. His research focuses on shape-controlled synthesis and self-assembly of metal and semiconductor nanocrystals for exploring their optical properties and optoelectronic applications. He serves on the Editorial Advisory boards of Nanoscale, Advanced Optical Materials, and Advanced Physics Research, and is a Topic Editor for ACS Energy Letters.

Invited Lectures

Exploring Methods to Control The Emission Properties of Double Perovskites

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Lead-free halide double perovskites (DPs) are emerging as alternate materials for optoelectronic applications. Efforts are on to understand the various mechanisms at play that are operational in influencing the optical and electronic properties of these materials. Transmuting two lead cations by a +1 and +3 cation enables the formation of $A_2B^{(I)}B^{(III)}X_6$ double perovskites. The luminescence of $Cs_2AgInCl_6$ can be enhanced upon incorporating a small amount of Al^{3+} or Bi^{3+} in the structure. The PL has been hypothesized to arise as a result of the self-trapped excitonic (STE) emissions. Understanding the structure of the STEs is most important in order to design materials with a handle to tune these properties. Doping of these DPs also results in energy transfer from the host to the dopants given that excited states of the two overlap, enabling the transfer. Further, as in the case of semiconductors, core-shell materials with the proper band alignments can be useful for controlling the optoelectronic properties.

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Bio-sketch

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Dr. Sameer Sapra is interested in the development of materials for energy conversion; photovoltaics and photocatalysis being the main forte. He obtained his doctorate in chemistry from the Indian Institute of Science, Bangalore working with Prof. DD Sarma on the electronic and optical properties of semiconductor nanocrystals in 2004. After completing his PhD, he was awarded the Alexander von Humboldt fellowship to carry out research on the luminescence properties of quantum dots at the Ludwig Maximilian University at Munich. From there he moved to the group of Prof. Dr. Alexander Eychmueller in Dresden. After researching for three years on the luminescence properties of quantum dots, Sameer moved back to India and joined the Indian Institute of Technology where he currently works on the various aspects of nanomaterials - his interests ranging from basic size and shape dependent studies, synthesis of new materials such as those based on transition metal dichalcogenides and perovskites, light emitting materials, photovoltaic devices and photocatalytic applications including hydrogen and oxygen evolution reactions. Along with research, he teaches various courses in Physical Chemistry and Materials Chemistry and mentors postdoctoral fellows, PhD, master and bachelor students.

Visible-Light Photocatalysis with Quantum Dot-Sensitized Photon Upconversion

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The dependence on high-energy UV light in photochemical reactions raises serious sustainability concerns due to its low natural abundance and its potential to induce undesired photodecomposition. Photon upconversion, especially triplet-triplet annihilation-based upconversion (TTA-UC), has emerged as a powerful strategy to access high-energy photochemical processes using visible or near-infrared (NIR) light.[1,2] Although molecular sensitizers have traditionally dominated TTA-UC systems, quantum dot (QD)-sensitized platforms offer distinct advantages, including strong and tunable optoelectronic properties, versatile surface chemistry, and spin-mixed energy states that enable larger anti-Stokes shifts.[3] Consequently, various QD-sensitized TTA-UC systems with excellent quantum yields and large photon energy gain have been developed.[4] However, the successful application of QD-sensitized UC energy in photocatalysis remains limited, especially for driving UV-demanding chemical reactions. Addressing this gap, our group has designed an InP QD-sensitized green-to-blue TTA-UC system exhibiting a normalized upconversion quantum yield of ~8.2 % and an anti-Stokes shift of 0.55 eV. Comprehensive steady-state and time-resolved spectroscopic studies confirm efficient triplet-triplet energy transfer and UC processes within the system. The UC energy was further used to carry out two important classes of UV-demanding reactions: (i) C-C coupling reaction via the dehalogenation of substituted aryl halides, and (ii) radical polymerization of methyl methacrylate (MMA) to produce the industrially valuable polymethyl methacrylate (PMMA).[5] These results highlight the potential of QD-sensitized TTA-UC systems in expanding the scope of visible-light photochemistry, thereby advancing in sustainable solar energy utilization.

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Bio-sketch

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Pramod P. Pillai is a Professor in the Department of Chemistry at the Indian Institute of Science Education and Research (IISER), Pune, India. His group's research is focused on controlling the interplay of forces to improve and impart newer properties at the nanoscale. Some of the properties of interest include light harvesting, catalysis, and self-assembly. He obtained his PhD in Chemistry from the National Institute for Interdisciplinary Science and Technology (NIIST), Trivandrum, India. Prior to joining IISER Pune, he was a postdoctoral fellow at Northwestern University, Evanston, IL, USA, and an Alexander von Humboldt postdoctoral fellow at Technische Universität ̈t, Dortmund, Germany.

Teaching Molecules to Change Colour: Lessons from Chem 101

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Photochromic molecular switches undergo reversible changes in their structure and electronic properties when exposed to light, giving rise to a dynamic behavior.[1] Tuning the photochromic properties of molecular switches with light provides a powerful approach to designing adaptive, stimuli-responsive materials for memory and logic materials.[2] Although this may sound complex, the design of these systems is rooted in simple principles of organic chemistry that are taught in undergraduate chemistry classes. We show how basic concepts from organic chemistry can be used to understand and precisely control the properties of these switches through light-driven isomerization processes.[3-6]

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Subhajit Bandyopadhyay teaches chemistry at IISER Kolkata. He is the founder of the IISER Kolkata Arts Club. He likes old buildings and monuments, reads history, and listens to old music on an old gramophone.

Controlling Photon Emission Statistics from Quantum Dots

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Classical light sources emit photons in a Poisson number distribution centered around a mean number.[1] In contrast, a single photon emitter emits a photon in a non-classical number state with a unit probability of emitting a single photon and a zero probability of emitting more than one photon in a single event. This form of non-classical emission is essential for a host of quantum applications.[2,3] Application of single photon emitters towards information processing system relies on their efficiency, fidelity and rapid cyclability. Amongst the many possible sources, quantum dots are considered most promising[4] even though real quantum dots still suffer from the multiphoton emission problem under non-ideal driving conditions. This presentation will describe our work towards realizing single photon emission from quantum dots and their assemblies.

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AP did his PhD from University of Chicago and is presently at the Solid State and Structural Chemistry Unit. He is interested in Spectroscopy and synthesis of nanocrystals.

Water-Enhanced Deep Eutectic Electrolytes for Stable Zinc-Ion Batteries

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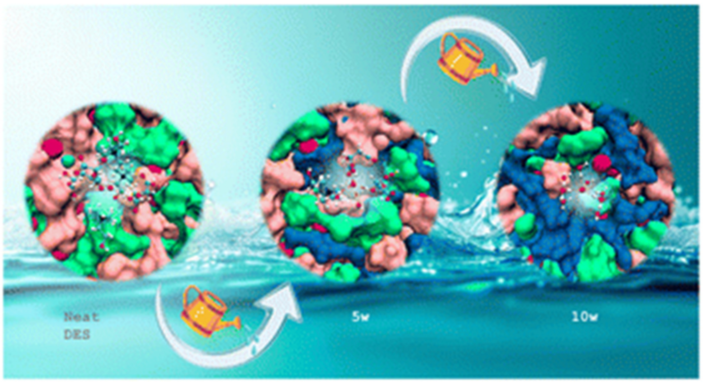
Aqueous Zn-ion batteries (ZIBs) are emerging as safer and more sustainable alternatives to traditional Li-ion batteries. Among the critical components of ZIBs, the electrolyte plays a key role in determining electrochemical performance and battery efficiency. However, conventional aqueous electrolytes pose challenges for Zn anodes, including poor reversibility and limited cycling stability caused by dendrite formation. To address these issues, "Water-in-Deep Eutectic Solvent (DES)" electrolytes have garnered attention as eco-friendly and cost-effective solutions. Despite their promise, fundamental questions remain unanswered: the optimal water content in DES, the effect of water on electrolyte dynamics, the disruption of DES hydrogen bonding networks, and the changes in the Zn^{2+} solvation structure in water-in-DES systems. Using ultrafast 2D IR and 2D NMR spectroscopy, we investigate solvent dynamics, structural rearrangements, and hydrogen bonding behavior across varying water concentrations, both with and without Zn salts. Complementing these experimental methods, molecular dynamics (MD) simulations provide insights at the molecular level. Our findings reveal that adding 10 moles of water per mole of DES optimizes electrolyte performance, as confirmed by peak conductivity in impedance spectroscopy. These results offer valuable insights into improving ZIB electrolytes and enhancing their practical applicability.



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Dr. Bagchi began his independent career at CSIR-NCL in 2012. His research group employs a combination of experimental and computational techniques to gain molecular-level spectroscopic insights into complex heterogeneous systems across chemistry, biology, and materials science. Key areas of investigation include dynamic heterogeneity in deep eutectic solvents, the role of water in liquid-liquid phase separation, surface-ligand interactions in quantum dots, and the mechanistic understanding of next-generation electrolytes.

Next Generation Dopants for Organic Electronics

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Organic conjugated compounds and halide perovskite materials are driving progress in low-cost optoelectronics. To expand their use, electronic doping is crucial. Typically, molecular and metal complex dopants are employed, but their high costs, limited efficiency, and stability issues necessitate alternative approaches. We have thus developed a variety of dopants suitable for numerous organic semiconductors, enabling effective and durable doping of organic transport layers in perovskite devices. We also showcase how this innovative doping technique can be applied in metal halide perovskite solar cells, organic thin-film transistors, and organic light-emitting diodes.

Bio-sketch

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Research Interest and expertise:

The Principal Investigator (PI) employs a materials-driven strategy for advancing optoelectronic devices, focusing on understanding and manipulating the underlying chemistry and physics that dictate material behaviour and device functionality. This approach is particularly critical in emerging technologies such as perovskite solar cells and flexible electronics, where material stability, interfacial control, and device architecture play interdependent roles.

Selected Awards and Honours:

1. DST Solar Challenge Award (2023)
2. Swarna Jayanti Fellowship (2021)
3. Infosys-TIFR- leading edge science fellowship (2021)
4. Associate Editor for MRS Energy and Sustainability, (2016- 2019)
5. Smart Solar UK award, Smart Solar UK (2016)
6. Feature Editor on Perovskites for MRS Bulletin, Materials Research Society (2015-till date)
7. Marie Skłodowska-Curie Fellowship, European Union (2015)
8. INSPIRE Faculty Award, Dept. of Science and Technology, Govt. of India (2013) (declined)
9. Dean of Faculty Fellowship, Weizmann Institute of Science, Israel (2011)

Citation index at Google Scholar, (Total citations: 9868 , h-index = 40)

Intracellular Subdegree Temperature Sensing and Dynamics by Thermoresponsive Silver Nanoclusters as Molecular Probes

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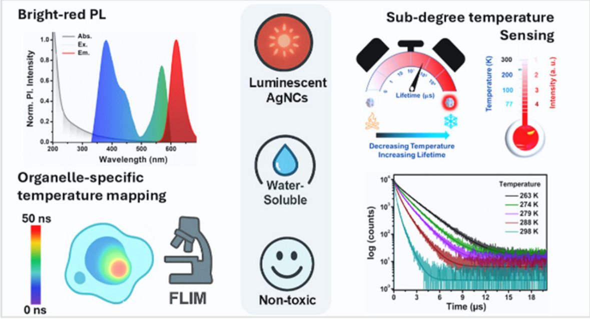
Noble metal nanoclusters (MNCs) have emerged as promising alternatives to organic dyes and quantum dots due to their robust stability, superior biocompatibility, and tunable physicochemical properties.[1,2] However, their full potential in theranostics, sensing, and biological imaging has yet to be realized. Here, we report long-lived, red-luminescent silver nanoclusters (AgNCs) stabilized by the small-molecule ligand thiolactic acid, which exhibit exceptional stability (shelf-life exceeding three years, photostability ~100%), water-solubility, and high biocompatibility, making them suitable for diverse applications such as sensing and live-cell imaging.[3] AgNCs display extremely sensitive (>2% K^{-1}) and reversible luminescence responses to temperature, enabling subdegree (<0.5 K) precision in local thermal mapping through simultaneous monitoring of emission intensity and excited-state lifetime. Cellular assays, including MTT viability tests, confocal fluorescence imaging, and fluorescence lifetime imaging microscopy (FLIM), suggest that the non-cytotoxic AgNCs specifically stain lysosomes in live mammalian cells, functioning as an organelle-specific biomarker and providing critical insights into lysosomal dynamics and intracellular temperature fluctuations.[3] The unique properties of these AgNCs, corroborated by detailed mechanistic studies, open new avenues for studying nanoscale subcellular physiology and developing temperature-sensitive diagnostics and preservation strategies.



The schematic representation of the work, reflecting the salient features of the present investigation.

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Bio-sketch

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Professor Mukherjee's research interests include ultrafast and single molecule spectroscopy of luminescent metal nanoclusters and self-assembled systems having biological relevance. He is the recipient of the INSA Young Scientist Award, CRSI Young Scientist Award, CRSI Bronze Medal and has been a Core and Founding Member of Indian National Young Academy of Sciences (INYAS). Professor Mukherjee is a Fellow of the Indian Academy of Sciences, Bangalore, the National Academy of Sciences, Allahabad, and a Fellow of the Royal Society of Chemistry. He is a Senior Editor of Chemical Physics Impact, a journal published by Elsevier. He has also served IISER Bhopal as its first Deputy Director.

Keeping The Chromophores Crossed for Efficient Photoinduced Symmetry-Breaking Charge Separation

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A comprehensive understanding of the structure–property relationships in multichromophoric architectures has pushed the limits for developing robust photosynthetic mimics and molecular photovoltaics.[1] Fascinatingly, Kasha predicted that the orthogonally cross-stacked molecular transition dipole arrangement would exhibit null exciton interaction, leading to a spectroscopically uncoupled molecular assembly that lacked an experimental signature for decades.[2] The elusive phenomenon of null exciton splitting has gathered immense attention in recent years owing to the occurrence in unique chromophoric architectures and consequent emergent properties. Symmetry-breaking charge separation is crucial in designing efficient organic photovoltaic devices by enhancing open-circuit voltage (V_{oc}) and thereby increasing power conversion efficiency. Herein, we explore photoinduced symmetry-breaking charge separation in orthogonally arranged perylenediimide dimers, providing impeccable evidence for the role of selective charge filtering in governing efficient SB-CS and offering novel insights towards the design of biomimics and advanced functional materials.[3,4]

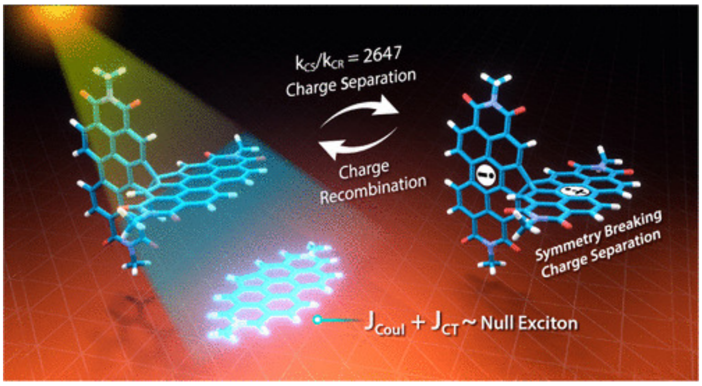

Figure 1: Symmetry-breaking charge separation in null-coupled spiro-bridged perylenediimide dimer.

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Bio-sketch

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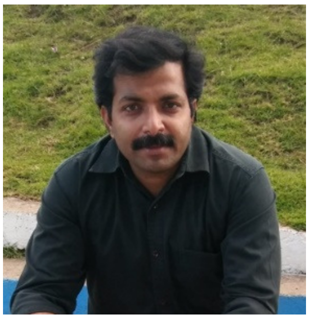

Mahesh Hariharan is a Professor at School of Chemistry, IISER Thiruvananthapuram. After completing doctoral research (2002-2007) from CSIR-NIIST India with Dr. D. Ramaiah, Dr. Hariharan carried out postdoctoral research (2007–2009) with Prof. F. D. Lewis at Northwestern University. His research efforts focus on understanding the interaction of light with biomolecules, crystalline and twisted organic materials.

Tailoring Molecular Structure for Optimized Singlet Fission

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Singlet fission is a multiexcitonic photophysical process in which a photoexcited singlet exciton splits into two triplet excitons within π-conjugated molecular systems. This conversion proceeds through an intermediate multiexcitonic state known as the correlated triplet pair (^{1}TT). In intramolecular singlet fission (iSF), covalently linked acene dimers have emerged as versatile platforms for modulating the electronic coupling between chromophores. A central challenge in iSF is achieving the optimal balance of electronic interactions. The chromophores must couple strongly enough to generate the ^{1}TT state, yet decouple sufficiently to enable efficient triplet separation.

In this talk, I will discuss molecular design principles and synthetic strategies that address this delicate balance. In particular, I will highlight how tuning the exchange energy and controlling torsional angles within acene dimers can serve as effective design handles to direct the dynamics of singlet fission.

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Satish Patil is a Professor at the Solid State and Structural Chemistry Unit, Indian Institute of Science (IISc), Bangalore. He did PhD in polymer chemistry with Prof. Ullrich Scherf at Bergische Universität Wuppertal. He did his postdoctoral work with Prof. Fred Wudl at the University of California, Los Angeles. His research work at IISc is primarily focused on investigating various aspects of molecular electronics, encompassing organic photovoltaics, Singlet Fission, and mixed-ion electronic conductors.

Probing Singlet Exciton Fission in Molecular Cyclophane Dimers

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Singlet fission (SF) is a process of multi-exciton generation in molecular aggregates where two independent triplet states are formed via an intermediate correlated triplet-triplet ^{1}TT pair state.[1,2] SF has been shown to occur within a minimal dimeric unit with chromophores having either monomer triplet energies that are half the allowed bright singlet state energy or hosting a multiexcitonic ^{1}TT state with enough stabilization compared to bright singlet state.[3,4] However one basic tenet of SF has always remained a challenge: What are the competing pathways that can reduce the quantum yield of extracted triplets? I will present our recent data on halogenated pentacene cyclophane dimers that demonstrates that inter-system crossing can still occur from the rich spin-physics of the multi-excitonic TT state if separation is not driven by thermal effects.[5]

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Bio-sketch

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Prof. Jyotishman Dasgupta received his 5-years Integrated Masters degree in chemistry from Indian Institute of Technology, Kharagpur in 2000. Subsequently he moved to Princeton University as a Hughes Stott Taylor graduate fellow where he carried out his Ph.D. work in the field of oxygenic photosynthesis under the supervision of Prof. G. Charles Dismukes. In 2006, he moved to UC Berkeley where he did his postdoctoral work with Prof. Richard A. Mathies. He joined the Tata Institute of Fundamental Research, Mumbai in 2010, and has been there ever since. The central theme of his research group is to probe dynamical structural events leading to charge generation in molecular materials, in order to fabricate bio-inspired molecule-based devices for photocatalysis and solar electricity generation. He received the 2017 Asian and Oceanian Photochemical Association (APA) Prize for Young Scientist, the 2018 Best Emerging Investigator Award and the 2024 CRS Silver Medal. He has been inducted as a Fellow in the Royal Society of Chemistry as "Leaders in Field", and has been in the editorial board of the major physical chemistry journals: *ACS Chemical Reviews, JPC Letters, Journal Physical Chemistry and Journal of Chemical Physics.*

Electronic Structure and Mechanism of Singlet Fission

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Mechanism of singlet fission and the design principles of the molecules that enhance it has long fascinated researchers. In this talk, I will explain some of the challenges of understanding the electronic structure of these processes. We will highlight the recent successes we have had.

The multireference methods that one needs to develop to understand these processes will also be discussed along with the variational versus machine learning methods that one can apply.

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Prof. Debashree Ghosh obtained her M.S. degree in Chemical Sciences from IISc in 2005 and PhD degree from Cornell University, USA in 2010. She joined CSIR-NCL as a Senior Scientist in 2012, subsequently moving to Indian Association for the Cultivation of Science. Currently she is a professor at IACS. Her research focuses on the development of polarizable force fields and their hybrid frameworks with excited-state electronic structure methods, geared towards understanding the photo-physics of biological systems. She has been recognized by several awards, including the Annual Medal of the International Academy of Quantum Molecular Science (2021), SERB-POWER fellowship (2022) and Walter Kohn prize awarded by International Centre for Theoretical Physics (2022).

Research Interests:

1. Photoprocesses of biological systems
2. Development of methods for strongly correlated systems

Awards and Honours:

1. Emerging Investigator Lectureship award, PCCP (2018)
2. Annual Medal of the International Academy of Quantum Molecular Science (2021)
3. SERB POWER Fellowship (2022)
4. Walter Kohn prize by ICTP, Trieste (2022)
5. Editorial advisory board member of IJQC, Electronic Structure, Phys Chem Chem Phys, Mol. Phys., Journal of Chemical Sciences, J. Phys. Chem., J. Chem. Theory Comput., Chem. Soc. Rev.

Visualizing Ribosomal-RNA Methylation Proteins in Action

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Förster Resonance Energy Transfer (FRET) in solution has been extensively utilized to determine proximity between fluorophore tagged to biomolecules and thereby probe intra or intramolecular structural changes. However, owing to ensemble averaging effect, solution FRET studies are inadequate to unveil real-time interaction dynamics between biomolecules or domain fluctuations therein. In contrast, single-molecule FRET (smFRET) measurements performed on a large number of individual surface immobilized biomolecule(s) labelled with donor and acceptor fluorophores can reveal intricacies of conformational dynamics and thus, provide new mechanistic insights. In our laboratory, we have assembled a smFRET setup which involves a total internal reflection fluorescence microscope (TIRFM) equipped with multiple lasers, coupled with a dual-channel image splitter placed before a CCD camera. This setup allows us to visualize the conformational dynamics of a large number individual biomolecules (proteins and nucleic acids) when immobilized on a surface. Here, I will discuss how we utilize smFRET to elucidate interactions between a bacterial ribosome – a complex protein-RNA machinery involved in protein synthesis – and a methyl transferase enzyme (Erm) during the methylation of a precursor ribosomal RNA (rRNA), a process which forms the basis for antibiotic (erythromyocin) resistance in a class of bacteria. While we rely on the Cryo-EM structural information on the complex between the Erm and immature ribosomes (*obtained by Ruchi Anand's group*), smFRET efficiency histograms and transition probability between various conformational states provide complementary information on the interaction dynamics between the enzyme and the precursor ribosome. Further, evidence of multiple conformation states and domain fluctuations of Erm subsequent to binding immature ribosomes provides a plausible mechanism of target search for (repeated) methylation of rRNA by Erm, a crucial (initial) step to confer antibiotic resistance to the bacteria.

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Bio-sketch

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Arindam Chowdhury obtained a BSc in Chemistry from University of Calcutta and a Masters from IIT Kanpur (1997), which was followed by a PhD (2003) in Chemistry from Carnegie Mellon University. After a post-doctoral stint at Columbia University, Dr. Chowdhury joined IIT Bombay in 2006 as an Assistant Professor, where he established a single-molecule fluorescence imaging, spectroscopy and dynamics laboratory for interdisciplinary research. Over the years, his research focus has been to elucidate origins of spatiotemporal heterogeneity in complex systems – soft-materials, semiconductor nanocrystals and perovskites, dynamics of biomolecular interactions – for which his group has developed both experimental and analyses methods. Prof. Chowdhury is currently affiliated with National Centre for Photovoltaic Research and Education (NCPRE), Wadhwani Research Center for Bioengineering (WRCB) and Center for Aging and Neurodegenerative diseases (SCAN) at IIT Bombay.

Polarization Engineering for Artificial Neural Circuits

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Neuromorphic computing architectures that emulate brain-like information processing offer transformative potential for developing energy-efficient artificial intelligence and next-generation in-memory computing systems. In this talk, we present two complementary strategies for realizing neuromorphic device functionalities using solution-processed organic and hybrid materials. The first approach leverages ionotronic mechanisms, where mobile ions within the active layer dynamically modulate the channel conductance, thereby mimicking short-term and long-term synaptic plasticity through ion migration and accumulation. The second strategy exploits ferroelectric polarization switching, in which the reversible alignment of electric dipoles induces non-volatile modulation of charge carrier density, leading to stable bi-stable states suitable for long-term memory and programmable synaptic weights. The devices exhibit robust memory retention and endurance, enabling effective handwritten pattern recognition. Overall, this work establishes a materials- and mechanism-driven framework for developing energy-efficient, non–von Neumann computing architectures that can bridge the gap between artificial and biological intelligence.

Bio-sketch

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Dr. Satyaprasad P Senanayak is a Reader in Physics at the National Institute of Science Education at Research (NISER), Bhubaneswar. He received his Ph.D. in Materials Science from JNCASR, Bangalore (2009 – 2015) for his work on developing high performance, low power, fast switching polymer field effect transistor. He then pursued his research at the Cavendish Laboratory, University of Cambridge working on developing Perovskite Field effect transistors. He was awarded the prestigious Royal Society Newton Fellowship, EPSRC Global Challenge Award, Royal Society Alumni Fellowship, Young Scientist Award of Odisha Bigyan Academy. He is a Early career member of American Physical Society, Associate of Indian Academy of Sciences and Member of Odisha Bigyan Academy. His current research at NISER addresses two focused areas: (a) Development of ferroelectric neuromorphic devices; (b) High performance perovskite field effect transistors.

Vibronic Phosphorescence and Thermally Stimulated Delayed Phosphorescence: A Theoretical Perspective

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The present talk will cover a range of theoretical methods to shed light on the origin of multi-peak vibronic phosphorescence that eventually leads to the realization white light Pholed. Using time dependent correlation function approach, we have developed a new code that can capture the vibronic feature of a phosphorescence spectrum and the photophysics behind the anti-Kasha behavior is then explained after evaluating the rate constants of various nonradiative processes that helps explain the origin of white light emission from the anti-Kasha molecules. It is worth noting that delayed phosphorescence is a relatively new phenomenon and here also the phosphorescence occurs from T_2 state with a prerequisite condition of T_1-T_2 reverse internal conversion. Till date, only a few molecules exhibit such interesting phenomenon. We know that phosphorescence is usually a second order process however T_1-T_2 reverse IC requires nuclear kinetic energy as an additional perturbation which makes delayed phosphorescence as third order process and a bit challenging at the theoretical level to address it. Recently we have developed a new third order perturbation theory that can successfully explain this amazing experimentally observed phenomenon (T_1-T_2-S_0 process).

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Swapan Chakrabarti is an associate professor of physical chemistry at the University of Calcutta. He received his PhD degree from the department of physics of the same University in 2001. As a visiting researcher, he has working experience in many renowned institutes and in particular, he has formed a very successful collaboration with Prof. Kenneth Ruud of Hylleraas Centre for Quantum Molecular Sciences, Norway. His current research attention is mainly focused on the theory of ultrafast quantum processes. He has published around one hundred scientific articles in journals of international repute. In 2010, he received a Distinguished Lectureship Award at the 90th annual meeting of the chemical society of Japan.

Ionic Liquids in The Synthesis and Photophysical Modulation of Semiconductor Nanocrystals

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Ionic liquids (ILs), comprising organic cations and organic or inorganic anions, constitute a versatile class of low-melting salts distinguished by negligible vapor pressure, high thermal and chemical stability, and tunable structural and functional attributes. These unique physicochemical properties have positioned ILs as "designer solvents" capable of providing tailored microenvironments for advanced materials synthesis. This talk will present our efforts in leveraging ionic liquids for the synthesis, stabilization, and photophysical modulation of perovskite nanocrystals, and will highlight their potential in nanomaterial design and optoelectronic applications.

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2. Chakraborty, D.; Preeyanka, N.; Akhuli, A.; Sarkar, M. Enhancing the Stability and Photoluminescence Quantum Yield of $CsPbX_3$ (X = Cl and Br) Perovskite Nanocrystals by Treatment with Imidazolium-Based Ionic Liquids through Surface Modification. *J. Phys. Chem. C* **2021**, 125, 26652–26660.
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Academic Background	Ph.D., University of Hyderabad, India (2007) M.Sc., Burdwan University, India
Professional Experience	Professor: NISER Bhubaneswar (2023) Associate Professor, NISER Bhubaneswar (2016) Reader-F, NISER Bhubaneswar (2012) Assistant Professor, NISER Bhubaneswar (2009)

Research Interests

Inorganic Nano Materials, Ionic Liquids.

Recent Publications

1. Probing Lithium-ion Induced Micro-environment Changes in Pyrrolidinium-Based Mono-cationic and Di-cationic Ionic Liquid. Amita mahapatra, Unmesh Dutta Chowdhury, Subhakanta Parida, Sahadev Barik, Joyoti Ghosh, B.L. Bhargava, Moloy Sarkar.* *Phys. Chem. Chem. Phys.* 2025, 27, 14777.
2. Surface-Controlled Modulation of Copper Nanocluster-DNA Interaction and Its Implication for Targeted Biological Applications, Joyoti Ghosh, Chinmayee Patra, Debabrata Chakraborty, Debraj Koiri, Sumit Kumar Pradhan, Moloy Sarkar.* *ACS Appl. Nano Mater.* 2025, 8, 21, 11150–11165.
3. Ionic Liquid Engineered Defect-Driven Green Emitting Zero-Dimensional Cs_4PbBr_6 Microdisks. Debabrata Chakraborty, Amit Akhuli, Moloy Sarkar.* *J. Phys. Chem. Lett.* 2025, 16, 37, 9646–9655.

Fluorescent Materials: Self-Assembly and Photocatalytic Applications

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Our research work aims at development of donor-acceptor building blocks which undergo self-assembly in aqueous media to generate fluorescent assemblies in aqueous media.[1-5] These assemblies having appropriate binding sites for interactions with specific analytes undergo guest induced morphology transformation and exhibit interesting photophysical properties. Very recently, we have developed supramolecular assemblies having chiral - handle and investigated the achiral/chiral guest induced chirality transformations in aqueous media.[4-5] Furthermore, we have also developed metal based as well as metal free supramolecular catalytic ensembles for carrying out various organic transformations. In the presentation, different aspects of development of these 'lighted' materials and their molecular recognition and catalytic applications will be discussed.

References:

1. Singh, A.; Kumar, M.; Bhalla, V. Minimizing Radiative and Nonradiative Energy Leakage in Red-Light-Absorbing Supramolecular Nanoassemblies to Boost Oxidative Photocatalytic Activity in Water. *Catal. Sci. Technol.* **2025**, *15*, 4024-4036.
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5. Kumar, G.; Kumar, M.; Bhalla, V. Controlling the Transition of Nanospheres to Superhelices in Aqueous Media by Using a "Smart" Pyrazine Building Block. *Angew. Chem. Int. Ed.* **2022**, *61*, e202207416.

Bio-sketch

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Vandana Bhalla received her Ph. D. in Organic Chemistry from Guru Nanak Dev University, Amritsar in 1998 under the supervision of Prof. Harjit Singh. She was a JSPS postdoctoral fellow at Tohoku University, Sendai, Japan during 2002-2004 and JST researcher in Aida Nanospace project with Prof. Takuzo Aida of University of Tokyo, Japan. She is presently working as Professor at Department of Chemistry, Guru Nanak Dev University, Amritsar, India. She has published more than 215 research papers in international journals and has delivered around 75 lectures.

Research Interests:

Research interests lie in the area of supramolecular material chemistry and catalysis.

Awards and Honors:

i. Fellow, Indian Academy of Sciences Bangalore w.e.f. January 1, 2025
ii. AV Rama Rao prize for Women in Chemical Sciences for the year 2025 awarded by Chemical Research Society of India, Bangalore.
iii. SERB-POWER Fellowship for three years from March 30, 2021-March 29, 2024
iv. INSA Teacher award for the year 2020.
v. Rajib Goyal Award for the year 2017 for contribution in Chemical Sciences by Kurukshetra University, Kurukshetra.
vi. Prof. S. S. Sandhu Endowment Award, for the year 2017 awarded by Indian Chemical Society for contributions in Chemical Sciences.
vii. First Shiv Nath Rai Kohli Mid-Career Best Scientist Award for the year 2018 for contribution in Chemical Sciences by Panjab University, Chandigarh 2018.
viii. Bhagya-Tara award by Panjab University for contribution in organic chemistry 2015.
ix. Thomson Reuters Research Excellence India Citation Award 2015. First women scientist in India to get this award. This award is given to Indian scientists whose recent papers represented the strongest research performance in their research area in terms of number of highly cited papers, total citations to these highly cited papers, or both.
x. Bronze Medal Awarded by Chemical Research Society of India (CRSI), Bangalore.

Positions Held:

1. Editorial Board Member, Asian Journal of Organic Chemistry.
2. International Advisory Board Member, Chemistry: An Asian Journal.
3. Associate Editor, RSC Advances (since 2015).

What Drives Structural Distortions in Two Dimensional Hybrid Halide Perovskites?

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The hybrid perovskites are of interest in recent times because of their multifarious nature. The close correlation between the structure and the ensuing properties requires an understanding of the factors that drive the structural distortions. These are well understood among the inorganic perovskites in terms of a geometric quantity dependent on the radii of the atoms making up the materials. However, this is more complex in the hybrid perovskites, where the molecule interacts with the inorganic cage. Considering the three dimensional members which are few in a number we had identified the factors[1] that determine the distortions. However, this becomes more complex in the context of the two dimensional perovskites where the number is large. In this talk I will present our recent results[2] in which we identify few descriptors and explore their correlations with the structural distortions.

References:

1. Mondal, D.; Mahadevan, P. Structural Distortions in Hybrid Perovskites Revisited. *Chem. Mater.* **2024**, *36*, 4254-4261.
2. Khuntia, S. K.; Maiti, K.; Mahadevan, P. (in preparation).

Bio-sketch

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Dr. Priya Mahadevan is a Senior Professor in the Department of Condensed Matter and Materials Physics at SN Bose National Centre for Basic Sciences. She received her PhD from the Department of Physics, Indian Institute of Science, Bangalore in 1999. Her research interests include modeling materials using a combination of ab-initio and model Hamiltonian methods. She is a fellow of the Indian Academy of Science, and The World Academy of Science. She is the recipient of the NASI SCOPUS young scientist award (2010), and the TWOWS award for young woman scientist in Physics/Mathematics in Asis-Pacific region (2010) and the MRSI medal (2014). She is also an Editorial Advisory Board member of Journal of Magnetism and Magnetic Materials and Journal of Solid State Chemistry.

Rashba and Excitonic Physics in Emerging Materials and Correlations with Light-Matter Interaction: A Computational Insight

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We have successfully correlated the Rashba splitting with Excitonic Radiative lifetime in lower dimensional condensed matter systems with different periodic confinements and interfacial configurations, which would certainly have tremendous impact in discovering the emerging optoelectronic materials based on the fundamental charge carrier recombination in the light matter interactions.[1-3] We have also envisaged the transition between Rashba, Rashba-Dresselhaus and Persistent Spin Textures in novel perovskite systems in the form of a quasi-2D confinement.[4] We continued our quest of Rashba splitting driven water splitting mechanism in inorganic perovskite materials.[5,6] The next part will be devoted to theoretical understanding of piezochromism, where hydrostatic pressure could be employed as an effective tool, giving rise to novel crystal structures and optical properties, while it has proven to be an alternative to chemical pressure.[7,8] Therefore, new functional materials with intriguing properties can be designed by exerting external pressure and strain. In this connection, the composition dependent transition between Frenkel Exciton to Wannier-Mott Exciton in inorganic perovskites will be discussed.[9] I will end my talk touching upon our recent successful endeavour of pre-intercalation mechanism in energy storage materials, as recently appeared in Nature Materials.[10]

References:

1. Kumar, D.; **Chakraborty, S.*** *Phys. Rev. B* **2025**, *112*, 125107.
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3. **Chakraborty, S.*** *et al. ACS Energy Lett.* **2017**, *2*, 837-845.
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9. Kaur, J.; **Chakraborty, S**.* *Small* **2025**, *21*, 2408919.
10. Luo, Y.; Handy, J.; Das, T.; **Chakraborty, S**.;* Banerjee, S.* *Nat. Mater.* **2024**, *23*, 960-968.

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Dr. Sudip Chakraborty is leading Materials Theory for Energy Scavenging (MATES Lab) group in India's premier theoretical research Institute Harish-Chandra Research Institute (HRI) Allahabad (Prayagraj), Department of Atomic Energy, Govt. of India. After completing his Ph.D. in collaboration between Bhabha Atomic Research Centre (BARC) and University of Pune, India, he moved to Max Planck Institute, Düsseldorf, Germany in March, 2011 as a Max Planck Postdoctoral Fellow. In February, 2013, he joined Materials Theory Division, Uppsala University, Sweden as a Førskare (Senior Researcher). Since March, 2019, he started leading his group firstly in Department of Physics of IIT Indore and later on in HRI from May, 2021 onwards. He has been awarded the **Rising Stars by ACS Materials Au 2021**, among 300+ nominations worldwide, while he is the sole recipient from India. He has been awarded **MRSI Medal - 2024** by Materials Research Society of India and **SMC Bronze Medal-2025** by Society of Materials Chemistry, India. He has become the Associate Editor of Springer-Nature Journal Graphene and 2D Materials, while he has been in the Editorial Board of Journal of Physical Chemistry A/B/C (ACS), Energy Advances (RSC), Electronic Structure (IOP), Chemistry of Inorganic Materials (Elsevier) His works are appeared in Nature Materials, PNAS, Physical Review B, Physical Review Materials, Materials Today, ACS Energy Letters, JACS, ACS Nano, ACS Catalysis, Angew. Chem., Advanced Materials, Advanced Functional Materials, Chem. Mater. etc. He has 194 International publications with total 8200 citations and 50 h-index (Google Scholar: https://shorturl.at/SBMRs).

Conductivity in Battery Electrolyte Systems: Roles for Solution Structure, Ultrafast Solvent Modes and Ion-Ion Motional Correlations

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A comprehensive understanding of ion transport in battery electrolyte systems requires elucidating the interrelation between microscopic solution structure, relaxation dynamics, and motional correlations of ions.[1,2] We have studied several such systems, both via theoretical + computational and experimental techniques, could generate important understanding regarding the roles of solution ultrafast mode and dynamic correlations among ion movements in regulating ionic conductivities in solution phase.[3] The role of water structure and residence times in the proximity of ions have also been found to play critical roles in controlling conductivity in aqueous systems,[2] while cosolvent's influence has been investigated in determining the optimal composition of a given binary host system.[4] Formation of ion-pairs and ion-aggregates, and their effects on conductivity in these systems have also been ascertained.[1,5] Some of these results will be presented and the physical chemistry aspects discussed in this talk.

References:

1. Mondal, A.; Kumbhakar, K.; Biswas, R.* Correlating Ionic Conductivity to Structure and Dynamics of Li-Ion Battery Electrolyte Systems: Raman Spectroscopy, Dielectric Relaxation Measurements, and Streak Camera Solvation Data Analysis. *J. Phys. Chem. B* **2024**, *128*, 11924−11937.
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4. Maity, N. C.; Mitra, S.; Biswas, R.* *J. Phys. Chem. B* **2025** (submitted).
5. Mondal, A.; Biswas, R.* *J. Chem. Phys.* **2025** (submitted).

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Professor Ranjit Biswas is one of the few scientists who performs experiments, develops theory, and uses computer simulations to generate an integrated understanding of chemical events occurring in a wide spectrum of environments. His research has led to significant insights into the physical chemistry of deep eutectic solvents, ionic liquids, binary mixtures, and cryoprotectants. He has published so far ~150 research papers in front-ranking, peer-reviewed international journals. 19 students have so far received Ph.D. degrees after working in the laboratory of Professor Biswas and several of them are already engaged in research and teaching as permanent faculty members in various institutions of India including IITs. Currently, 4 PhD students and 2 post-doctoral fellows are working in the research group of Professor Biswas.

Prof. Biswas obtained his BSc and MSc degrees in Chemistry from the University of Kalyani (1990 & 1992 respectively), and PhD (1998) from the Indian Institute of Science, Bangalore, in Theoretical Physical Chemistry after working with Professor Biman Bagchi as his Thesis Supervisor. Prof. Biswas then spent 4 years in the laboratory of Professor Mark Maroncelli, Pennsylvania State University, where he learned experiments employing ultrafast laser spectroscopy. Professor Biswas is currently a Senior Professor and Dean (Academic Program) at the S. N. Bose National Centre for Basic Sciences (joined in 2002 as a Faculty Fellow), and an elected Fellow of the National Academy of Sciences (FNASc.), Allahabad.

Mapping Ultrafast Relaxation Dynamics of Large Stokes Shift Red Fluorescent Proteins

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While excited-state proton transfer (ESPT) underlies the bright fluorescence from wild-type green fluorescent protein, the large Stokes shifts in certain red fluorescent proteins (LSS-RFP) imply a more intricate excited-state photophysical behavior[1]. Our earlier work showed that mKeima[2] exhibits dual emission only at 77 K, a similar trend was also observed in LSSmKates[3]. In contrast, mBeRFP[4,5] displays dual emission at room temperature and triple emission at 77 K, the first reported example of triple emission in a fluorescent protein. To gain insight into ultrafast relaxation of different conformers in excited state, we carried out femtosecond transient absorption spectroscopy (fs-TAS) studies in both normal buffer and deuterated buffer. This work demonstrates the key role of ESPT in LSSmKate1 and LSSmKate2, which differ by a point mutation, and reports temperature-sensitive local and distant emissions, including dual and triple fluorescence in mBeRFP. Combining the results, we conclude that the branching of excited-state population through multiple conical intersections leads to LSS in LSS-RFP. The results are further supported by electronic structure calculations.

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Dr Arijit K. De completed his BSc (2003) from the University of Calcutta and and MSc (2005) from IIT Kanpur. He pursued his PhD with Prof Debabrata Goswami at IIT Kanpur (2005-2010), working on two-photon fluorescence microscopy and optical trapping. He was a postdoctoral fellow at the University of California Berkeley (CA, USA) with Graham R. Fleming (2010-2014), where he developed two-dimensional fluorescence-detected coherent spectroscopy (2D-FDCS). In 2014, he joined IISER Mohali (PB, India), where he is now an Associate Professor in the Department of Chemical Sciences.

The central theme of research in the “Condensed Phase Dynamics” group at IISER Mohali, led by Dr. Arijit K. De, is to explore, through a combination of experiments and theories, a multitude of multidisciplinary problems spanning chemistry, biophysics, and condensed matter physics.

The main focus of the group is to investigate energy and charge (electron/hole or proton) transfer dynamics, covering a wide range of timescales (a few tens of femtoseconds to a few nanoseconds), within systems of varying complexities (namely, organic chromophores and their aggregates/multichromophoric systems, transition metal complexes, halide perovskites, and fluorescent proteins), and the effect of the local environment (for example, solvation and nanoscale confinement) on it. To study these problems, the group developed a couple of cutting-edge spectroscopic techniques beyond widely used and commercially available femtosecond pump-probe (or transient absorption) spectroscopy, i.e., ‘two-dimensional electronic spectroscopy’, and ‘(time-resolved) impulsive Raman spectroscopy’, each of which is the first of its kind developed in India.

The group also pioneered in deciphering the role of optical and thermal nonlinearities in laser trapping under femtosecond pulsed excitation. Quite recently, they developed a ‘laser beam-shaping (with computer-generated holograms)’ apparatus to study the effect of orbital angular momentum in laser trapping and interactions between active/passive colloidal particles.

Halide Perovskite Nanomaterials for Energy and Optoelectronic Applications

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Halide perovskites have been rapidly expanding their applications from energy harvesting and usage to smart optoelectronic applications. While bulk materials are widely used in solar photovoltaic and detector applications, perovskite nanomaterials have been utilized in light-emitting diodes, photoluminescence, photo-rechargeable supercapacitors, memory, and neuromorphic applications. We have demonstrated a stable perovskite electrode-based photo-rechargeable supercapacitor fabricated from perovskite nanocrystals, therefore improving charge storage capacity. We have demonstrated that nanostructured perovskites exhibit enhanced electronic properties under illumination. Perovskite nanocrystals exhibit hysteresis under applied bias, thereby enhancing the memory effect in these devices. I will finally demonstrate that one of the key aspects in this area of research is the manipulation of electrical conductivity. We have demonstrated that conductivity can be simultaneously manipulated by tuning the gate-voltage characteristics and optical excitation in the channel. Therefore, mixed input logic operations can be visualized in single-layered perovskite devices, where both optical and electrical inputs can be tuned. Ultimately, we have demonstrated some of the basic logic operations, including NOT-gates, AND-gates, OR-gates, and XOR-gates, which are voltage-tuneable and compatible with neuromorphic computing. The inherent memory effect in these materials can be a blessing in disguise.

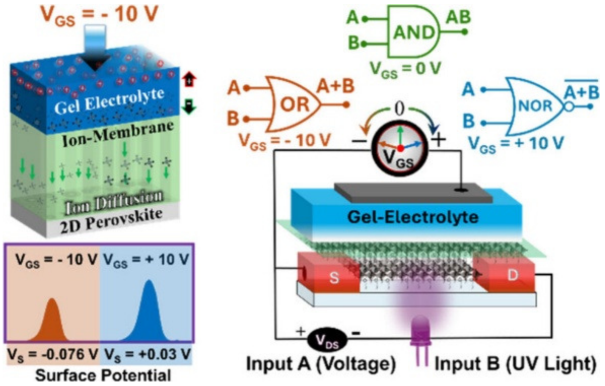

Figure 1: Voltage tuneable three-terminal logic gates demonstrating OR, AND, and NOR operations.

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Dr. Bag is currently an associate professor of the Department of Physics and an adjunct faculty member of the Centre for Nanotechnology at the Indian Institute of Technology Roorkee, India. He got his bachelor's degree in electrical engineering from Jadavpur University and his master's degree in physics from the University of Pune in 2003 and 2006, respectively. After completing his PhD at the Jawaharlal Nehru Centre for Advanced Scientific Research, India, in the field of Materials Science in 2011, he spent several years in postdoctoral work at the University of Massachusetts Amherst, USA, and at Lund University, Sweden, before joining IIT Roorkee in 2016.

Dr. Bag has worked on multi-disciplinary projects during his PhD and postdoctoral work with multiple research groups. His expertise spans device fabrication to various characterizations, including theoretical modelling and simulations. He has been working in the field of organic electronics for the last twenty years and has focused on hybrid perovskite-based materials for energy harvesting, storage, and other optoelectronic applications for the last twelve years. Some of his PhD and postdoctoral work have led to patents that have either been granted or filed. Artificial retina devices and polymer nanoparticle-based solar cells fabrication are among them. His current research highlights are halide perovskite-based high-performance supercapacitors, photo-rechargeable supercapacitors, memristors, and mixed-input universal logic gates. He has published over 80 research papers and several book chapters on related topics. Apart from research, he has been actively involved in teaching several courses related to energy and nanotechnology to undergraduate and postgraduate students. His current research laboratory, known as Advanced Research in Electrochemical Impedance Spectroscopy (AREIS) at IIT Roorkee, focuses on impedance spectroscopy measurements of various optoelectronic materials, as well as the fabrication and optimization of large-area thin-film-based solar cells and LEDs.

Polymer Perovskite Composites for Energy Harvesting Applications

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Hybrid inorganic-organic perovskites are among the most sought-after materials for a diverse range of applications, including solar cells, X-ray scintillators, light-emitting diodes, electrochromic devices, photodetectors, sensors and photocatalysts. Owing to exponential growth in 5G and IoT technologies, the need for integrable and efficient energy conversion devices is increasing. This allows the use of piezoelectric nanogenerators (PENGs) as smart, wireless, portable electronic systems and sensors. The devices leverage the piezoelectric properties of perovskite materials to convert mechanical stimuli into electrical signals. In this presentation, we show that the α–$FAPbI_3$ (perovskite phase) can be stabilized at room temperature, employing polymer additive engineering to form the $FAPbI_3$–Polymer composite. By employing excess halide (AX) alongside a polyvinylidene difluoride (PVDF) host, both surface passivation and spatial confinement occur during co-crystallization. Investigations on the interactions between the -CF_2 dipole of PVDF, the coordination-unsaturated Pb^{2+} defects, and the passivation of the shallow halogen vacancies in perovskites without disrupting their crystallisation. The co-crystallisation of electroactive polymers in conjunction with low-dimensional metal halides is a promising approach to co-passivate, quantum-confine, and spatially trap excitons, leading to a composite material system with ultra-bright luminescence, near unity PLQY, and significantly reduced thermal quenching. The free-standing film remains stable even after a year under ambient room conditions. Along with this, we show that using lead free alternatives, the polymer composites can be used to make self-powered sensors.

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Prof. Aswani Yella's research interests span the rational design, synthesis, and mechanistic understanding of molecular and hybrid functional materials for solar energy conversion and optoelectronic devices. Her work primarily focuses on interface engineering, and light-harvesting strategies in perovskites, and emerging photoelectrochemical systems. Motivated by the broader challenges in next-generation optoelectronics, her research has increasingly expanded toward light-emitting devices (LEDs), photodetectors, and solid-state architectures using perovskites, quantum dots, and 2D hybrid materials. Her group explores structure–property relationships in emissive nanomaterials, defect tolerance, carrier confinement, and exciton management to improve external quantum efficiency and spectral tunability in LEDs. In parallel, she is developing high-responsivity, low-noise photodetectors by engineering band alignment, charge extraction layers, and dielectric confinement effects in ultrathin semiconductor platforms.

Prior to joining IITB, Yella has carried out research on the synthesis of various nanomaterials, quantum dots and applied the synthesized different materials for photovoltaic applications. During the doctoral studies at Johannes Gutenberg University in Mainz under the guidance of Prof. Wolfgang Tremel, she has developed new synthetic routes for the synthesis of various chalcogenide nanomaterials for optoelectronic applications. During the post-doctoral studies at the laboratory of photonics and interfaces EPFL, Switzerland, she received "EPFL Prestations d´une Valeur Exceptionnelle" award for the year 2011, awarded by the Dean, Faculty of Sciences at EPFL. She joined the department of metallurgical engineering and materials science, Indian Institute of Technology – Bombay in April 2015. She has also been selected by the American Chemical Society as the Energy & Fuels 'Rising Stars'.

Developments in Cartesian-Grid-Based DFT in Atoms and Molecules (InDFT)

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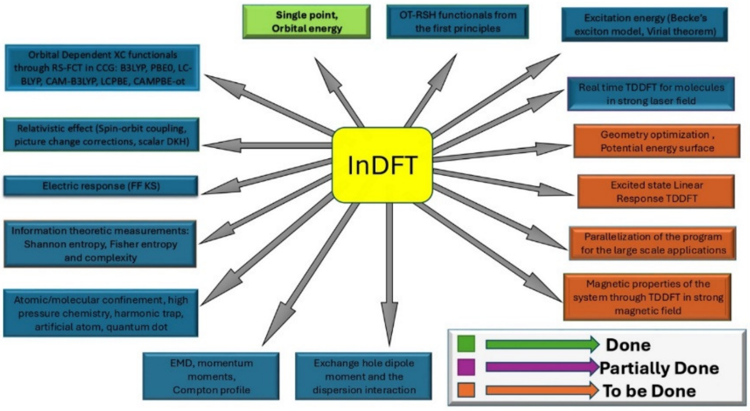
Density functional theory (DFT) has become a key participant in a phenomenal array of disciplines, from organic chemistry to condensed matter physics, over the past few decades. Here, we discuss some advancements made in our laboratory over the past few years. Through the use of a pseudopotential Kohn-Sham (KS) DFT framework based on a Cartesian coordinate grid (CCG) and the LCAO-MO ansatz, efforts are made to validate a viable alternative for DFT calculations for small to medium systems. To legitimize its suitability and efficacy, at first, electric response properties, such as dipole moment (μ), static dipole polarizability (α), first hyperpolarizability (β) are computed. Next, we present a purely numerical approach in CCG, to efficiently compute the exact contribution of exchange density in certain types of orbital-dependent density functionals.



A Fourier convolution theorem, combined with range-separated Coulomb interaction kernel is invoked. The inspiration for this came from a semi-numerical approach where the assessment of electrostatic potential determined the rate. Its success further leads to a systematic self-consistent approach from first-principles, which is desirable in the development of optimally tuned range-separated hybrid and hyper functionals. We then go over an alternate time-independent DFT method using the "adiabatic connection theorem" and the "virial theorem" to compute single-particle excitation energies. Optical gaps in organic chromophores, dyes, linear/non- linear PAHs, charge transfer complexes are accurately simulated. We then provide a novel method towards RT-TDDFT using TD KS equations based on an adiabatic eigenstate subspace (AES) procedure. To implement the approximate TD propagator in AES, it provides a second-order split operator approach. Apart from that, we also report results for a host of information theoretic measures, such as Shannon entropy, Fisher information, Rényi entropy, Onicescu energy as well as statistical complexity in both position and momentum space. Lastly, we report representative results on some momentum-space properties as well as Compton profile on atom/molecule. Also some progress is made on the quantum confinement and dispersion interaction in atoms/molecules. In summary, CCG-DFT is demonstrated to be an effective path for a variety of real-world applications in electronic systems.

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Dr. Amlan K. Roy completed his PhD in theoretical chemistry from Panjab University, in India. Later he pursued his post-doctoral research in a number of places in North America, such as University of New Brunswick (Fredericton, Canada), University of Kansas (Lawrence, USA), University of California (Los Angeles, USA), University of Florida (Quantum Theory Project). His primary research interest is to develop methods for electronic structure and dynamics of many-electron systems, within the broad domain of density functional framework. Presently he is Professor at IISER Kolkata. He has published more than hundred research papers and book chapters in reputed journals. He has been serving as a reviewer in many renowned journals. His biography has been included in 63rd Edition of Marquis Who's Who in America, 2009. In 2012 he has edited a book entitled "Theoretical and Computational Developments in Modern Density Functional Theory" and in 2024, he has edited a book entitled "A closer look at the Hydrogen atom".

Short Talks

Circularly Polarized Luminescent Nanomaterials and Assemblies: Exploring Optical Activity at The Nanoscale

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Chirality is ubiquitous in nature and chiral molecules/materials are finding application in diverse fields. This field of research has gained revived interest after the observation of optical activity in nanomaterials. Chiral nanomaterials are synthesized by adopting majorly three approaches: (i) the synthesis of intrinsically chiral nanoparticles in solution, (ii) chiral induction in achiral nanoparticles using chiral ligands, and (iii) template assisted methods using chiral/helical templates. Investigations on molecular chirality using circular dichroism (CD) spectroscopy has been an active research topic over the past few decades. Recently, research interest has focused attention on chiral light emitting molecules and materials due to their vast application in field of display devices, data encryption, chiral biosensing and bioimaging. CPL is a relatively new technique that has gained tremendous attention due to its relevance to both fundamental and applied research. Working in this direction, we have recently demonstrated CPL in organic molecular systems as well as nanomaterials. Our recent attempts towards understanding the fundamentals of optical activity in nanomaterials and the correlation of the observed spectral properties to the conventional organic systems will be discussed briefly. The potential applications of the nanomaterial systems will form the topic of discussion.

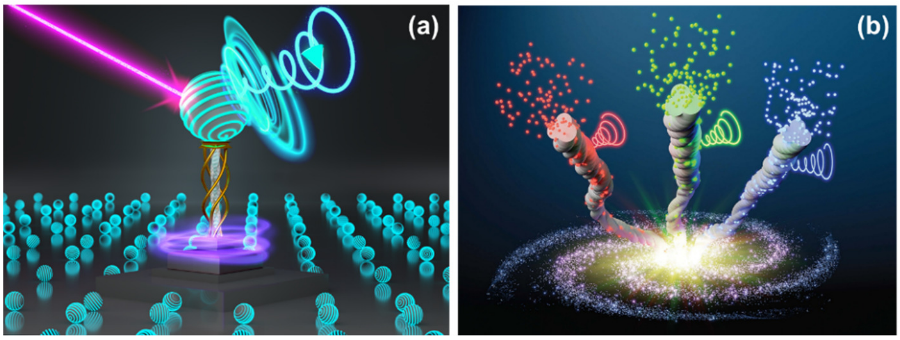

Figure: Scheme illustrating the chiral light emission in nanomaterials through (a) structural symmetry breaking and (b) host-guest interactions.

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Jatish Kumar is an Associate Professor in the Department of Chemistry at the Indian Institute of Science Education and Research (IISER) Tirupati. Jatish obtained his PhD in 2013 from CSIR-NIIST, Trivandrum working under the guidance of Professor K. George Thomas. Subsequently, he joined Prof. Tsuyoshi Kawai's group as a JSPS postdoctoral fellow at Nara Institute of Science and Technology (NAIST) in Nara, Japan. In 2016, he moved to CIC biomaGUNE, San Sebastian, Spain as a Marie Curie postdoctoral fellow to work with Prof. Luis M. Liz-Marzan. In December 2018, he began his independent career as an Assistant Professor at IISER Tirupati.

Jatish is a physical chemist with a research focus on materials science. His research interests include synthesis, characterization, and photophysical investigations of organic, inorganic, plasmonic and luminescent nanomaterials. Currently, the work in the group is focused towards understanding the ground and excited state chirality of various nanosystems. Special emphasis has been on the development of chiral light emitting materials to find application in display devices, security tags and biosensing. He has been on the Editorial Advisory Board of journals ACS Materials Letters and ACS Applied Optical Materials.

Enhancing Plasmonic Photocatalysis Through Ligand Engineering

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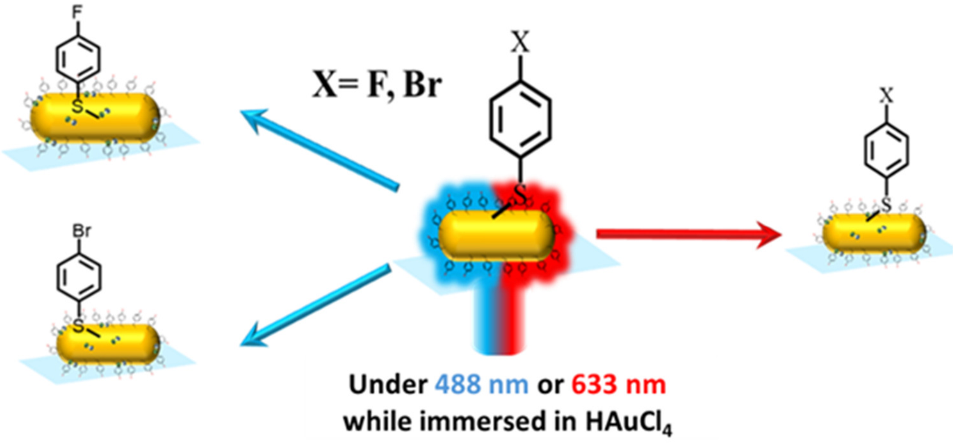
Plasmonic nanoparticles have the remarkable ability to convert photons into highly energetic charge carriers, making them promising candidates for light-driven catalytic transformations.[1] However, their practical efficiency is often limited by the ultrafast recombination of these carriers within the metal. In our study, we employed both bulk and single-particle spectroscopy to demonstrate that functionalizing plasmonic nanoparticles with specifically substituted thiophenol ligands can substantially enhance their photocatalytic efficiency.[2] Notably, under interband excitation, gold nanorods functionalized with 4-fluorothiophenol (Au-FTP) exhibited a photoreduction rate of Au^{3+} ions that was approximately 32 times higher than that of nanorods functionalized with 4-bromothiophenol (Au-BrTP). Interestingly, this dramatic difference was not observed under intraband excitation, where both types of functionalized nanorods showed minimal reactivity. Further theoretical and experimental investigations revealed that the enhanced rate under interband excitation arises from efficient hole transfer from the gold d-band to the HOMO of 4-FTP, which facilitates charge separation and leaves electrons available for the reduction of Au^{3+} ions. These findings highlight the crucial role of organic ligand design in promoting charge separation and provide a mechanistic framework for the rational development of efficient plasmonic photocatalysts.



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Bio-sketch

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I am an Associate Professor in the Chemistry Department at IIT Gandhinagar. I earned my Ph.D. from Rice University, USA, followed by a postdoctoral tenure at Leiden University, Netherlands. Since joining IITGN in 2015, we have established a cutting-edge optical microscopy and spectroscopy laboratory focusing on understanding the interactions between light and nanoparticles at single-particle concentrations. Our group focuses on developing plasmonic photocatalysts that efficiently convert solar energy into chemical fuels by generating and utilizing energetic hot carriers to drive chemical reactions. The hot carriers, possessing energies significantly above thermalized states, can drive demanding chemical transformations but are limited by rapid recombination. Our research focuses on overcoming this fundamental limitation by engineering plasmonic catalysts that enhance charge carrier utilization in a chemical process. Our research also expands to quantum dots and perovskite nanocrystals, improving their photostability and emission for optoelectronic applications through ligand and structural optimizations.

Tuning Peptide Secondary Structure on Gold Nanoparticles Through Controlled Thiol and Carboxylate Functionalization

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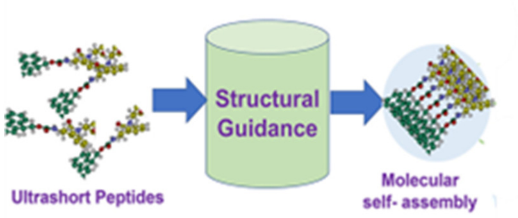
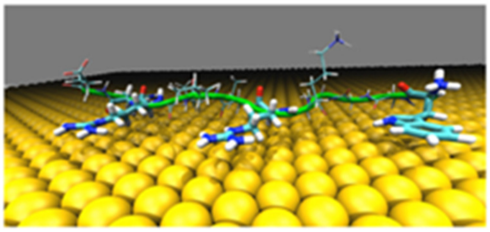
Understanding how peptides organise on metal nanoparticle surfaces is essential for designing functional nanomaterials with controlled stability, architecture, and biological activity. In this study, we investigate how the oxidation state of sulfur and the arrangement of terminal functional groups govern peptide secondary-structure formation on gold nanoparticles. Circular dichroism (CD) analysis of reduced and oxidised glutathione (GSH) revealed that free thiols promote flexible, random-coil structures through strong Au–S chemisorption, whereas disulfide-linked GSH, which adsorbs primarily through free carboxylate groups, adopts well-defined β-sheet conformations. To validate this structure–function relationship, we synthesised a series of model peptides with systematic variations in terminal –SH and $-COO^-$ groups. Mass spectrometry confirmed peptide identity, while CD spectroscopy demonstrated that peptides containing internal amide linkages and second-terminal thiols formed ordered β-sheet structures upon adsorption to gold. In contrast, peptides with two terminal –SH groups displayed dual behaviour: they assembled into parallel β-sheets in solution via intra- or intermolecular disulfide formation but reorganised into antiparallel β-sheet structures when adsorbed onto gold nanoparticles, where free carboxylates facilitated surface anchoring. Density functional theory (DFT) calculations supported these observations, showing stronger Au–S binding energies relative to $Au-COO^-$ interactions, highlighting the balance between strong chemical anchoring and conformational freedom in determining secondary structure. Overall, this work establishes how strategic modulation of peptide terminal functionalities can direct nanoscale packing, β-sheet arrangement, and adsorption behaviour, offering a rational route to engineer peptide–nanoparticle conjugates for drug delivery, biosensing, and biomimetic interface design.





Bio-sketch

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Academic Credentials

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  18th March, 2024-Continuing
- **DST INSPIRE Faculty**
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  1st January, 2019-14th March, 2024
- **Postdoctoral Researcher** with **Prof. Lev Chuntonov**
  Department of Chemistry, Technion-Israel Institute of Technology
  [Worked on **Two-dimensional Infrared Spectroscopy**]
  May, 2016- December, 2018
- **Postdoctoral Researcher** with **Prof. Jyotirmayee Dash**
  Department of Organic Chemistry, Indian Association for the Cultivation of Sciences (IACS), Kolkata, India
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PhD in Chemistry, (23/06/2015) Indian Institute of Science Education and Research Kolkata (IISER-Kolkata), West Bengal, India

Thesis title: Optical Spectroscopic investigation of nanoscopic environment in neat room temperature ionic liquids and in presence of dissolved solutes

***PhD supervisor*: Prof. Prasun K. Mandal**, Department of Chemical Sciences, IISER-Kolkata.

Exciton-to-Biexciton Transitions and Energy Transfer Dynamics in Mn-doped Perovskite Nanocrystals

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Understanding ultrafast exciton dynamics in doped perovskite nanocrystals (NCs) is crucial for advancing optoelectronic applications.[1] We studied the exciton-to-Mn dopant energy transfer dynamics in Mn-doped $CsPbCl_3$ NCs by looking at various spectral positions, which includes bleaching and photoinduced absorptions.[2] We reveal that the photoinduced absorption features, often overlooked, originate from exciton-to-biexciton transitions and provide a more accurate measure of exciton-to-Mn energy transfer dynamics. By analysing the bleaching and photoinduced signals we provided a detailed understanding of the slow energy transfer and Auger processes. Importantly, taking advantage of the slow exciton-to-dopant energy transfer process, we dissociated the exciton in Mn-doped perovskites via ultrafast electron shuttling to a surface adsorbed 4-nitro phenol molecule.[3] Our result suggest that the ultrafast electron shuttling sets a complete restriction to the exciton scattering and slow exciton-to-dopant energy transfer processes.

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Dr. Debnath is presently working as an assistant professor at the Department of Chemistry, Shiv Nadar University, Delhi NCR. He obtained his Ph.D. in Chemistry in 2016 from BARC, Mumbai, India. Subsequently, he moved to NTU, Singapore (2016 - 2018) as a postdoctoral fellow followed by LMU, Munich, Germany (2018 - 2022). He was Alexander von Humboldt fellow and optical spectroscopy group leader at the Department of Physics, LMU from 2019 – 2022. He started his independent research group, initially at IIT Guwahati, India (2022 - 2024) as a Ramanujan fellow and then at SNU Delhi NCR (2024 – present). Dr. Debnath is an expert in the field of optical and ultrafast spectroscopy of semiconductor nanocrystals and quantum dots. His present research interest focuses on the investigation of the fundamental photophysics of semiconductor and plasmonic nanomaterials, e.g. perovskite, chalcogenide nanocrystals, and plasmonic nanomaterials, primarily for energy-related applications. He has co-authored ~75 peer-reviewed publications of international journals of repute.

Young Investigator’s Flash Presentation

Self-Trapped Excitons with Unusually Large Huang-Rhys Factor in Halide Double Perovskite Semiconductor $Cs_2AgInCl_6$

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Lead-free halide double perovskites have emerged as promising optoelectronic materials with potential applications in photovoltaics and lighting technologies.[1] These compounds share a common chemical formula $A_2MM'X_6$. Here, A is a monovalent cation, M and M' are a monovalent and a trivalent metal ion, respectively, and X is a halide ion. Their soft polar lattices exhibit strong electron-phonon coupling, which favors the formation of self-trapped excitons (STEs) and leads to broad photoluminescence (PL) spectra.

Under 375 nm excitation, $Cs_2AgInCl_6$ single crystals display a bright, broad emission centered around 500 nm below 150 K [Figure 1(a)]. This is consistent with a previously identified STE emission. As the temperature increases, the PL peak undergoes an abrupt redshift to approximately 580 nm, which persists up to room temperature [Figure 1(a)]. Such a shift is surprising because powder X-ray diffraction [Figure 1(c)] and polarized Raman scattering confirm the absence of any global structural phase transition across this temperature range. A large linear thermal expansion response [Figure 1(d)], and increased phonon anharmonicity suggests that the observed spectral shift arises from thermally activated changes in the local lattice environment which modifies the electron-phonon coupling. These findings provide insight into the exciton–phonon interactions in lead-free double perovskites and offer a way to tailor their optical properties.

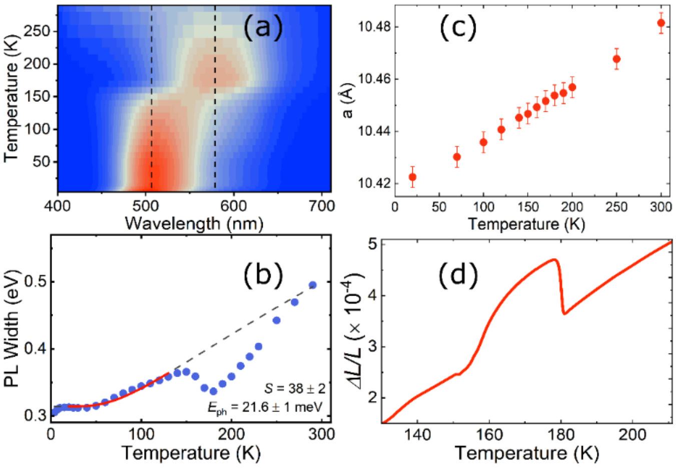

Figure 1: (a) Temperature-dependent evolution of the PL spectra of $Cs_2AgInCl_6$ single crystals under continuous-wave (CW) excitation at 375 nm. (b) Temperature-dependent broadening, $\Gamma(T)$, of the PL spectra, used to estimate the Huang-Rhys factor (S) by fitting with the equation $\Gamma(T) = 2.36\sqrt{S}\,\hbar\omega\sqrt{\coth\left(\frac{\hbar\omega}{2k_BT}\right)}$. (c) Lattice parameter (a) estimated from powder XRD measurements. (d) Linear thermal expansion behavior of $Cs_2AgInCl_6$ single crystals.

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EXPERTISE AND EXPERIENCE:

To investigate the interplay of charge, spin, orbital and lattice degrees of freedom one needs to often push the materials to extreme conditions like ultralow temperatures, very high pressures, bright radiation, and strong magnetic fields. I study semiconducting materials with spectroscopic tools and techniques by combining those conditions to explore interesting physical phenomena.

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Postdoctoral Researcher November 2025 - present
Research Topic: *Doped halide double perovskites as spin qubit candidates*
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Non-Covalent Reversibly Photoswitchable Fluorescent Tags for Wash-Free Protein Labelling

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Deciphering the complex mechanisms that govern cells and organisms requires fluorescent probes and real-time imaging techniques with high spatiotemporal resolution.[1] Consequently, major efforts have been devoted to developing new fluorescent probes and imaging technologies. In recent years, reversibly photoswitchable fluorescent proteins (RSFPs) have emerged as powerful probes, enabling advanced imaging modalities such as RESOLFT and LIGHTNING, which exploit their photoswitching behavior under illumination.[2] Herein, we introduce a series of new dark photoisomerizable fluorogens which, when combined with engineered protein scaffolds[3] (FAST/pFAST tags), yield the first representative of non-covalent reversibly switchable fluorescent proteins (ncRSFPs). Our strategy integrating thermokinetic, photochemical, and structural analyses provides an in-depth modelling framework for ncRSFPs. Leveraging our theoretical analysis, we reveal in living and fixed cells an unprecedented dual behavior of ncRSFPs driven by endogenous fluorogen interactions: from a wash-free fluorescent labeling tag to a negative reversible photoswitcher triggered by elevated light intensity and reduced fluorogen concentration. Finally, the versatility of these ncRSFPs is demonstrated through dynamic contrast and super-resolution imaging applications.

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Dr. Mrinal Mandal is a Postdoctoral Researcher at École Normale Supérieure (ENS), Paris, working in the group of Prof. Ludovic Jullien. He obtained his PhD in 2021 from IISER Kolkata under the supervision of Prof. Prasun K. Mandal, where he focused on developing small-sized Charge transfer fluorescent dyes with enhanced photophysical properties to image nano-polarity of live cells. His current research focuses on designing and developing Photoactive Probes and Non-covalent Reversibly Switchable Fluorescent Proteins (RSFPs) for dynamic contrast and super-resolution microscopy. Dr. Mandal has authored 16 peer-reviewed publications in high-impact journals and holds three patents. He has been recognized with the European Commission's Seal of Excellence award for his MSCA proposal. His broader expertise spans synthetic chemistry, photophysics, optogenetics, fluorescent labelling of proteins, and live-cell imaging. He aims to translate molecular innovation into new tools for visualizing and manipulating dynamic biological processes.

Interfacial Photophysics of Solar Cells with Non-Invasive Correlative Microscopy

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The interfaces within solar cells play a pivotal role in governing their performance, and long-term stability. Although device efficiency is commonly evaluated through macroscopic photophysical and electrical measurements, these bulk characteristics arise from intricate microscopic interactions occurring at buried interfaces where structural, chemical, and electronic properties converge. Defects, carrier transport pathways, and interfacial chemical reactions—particularly under operational stimuli such as light, bias, and ambient exposure—critically determine device functionality. This influence is especially pronounced in halide perovskite systems, whose soft and dynamic nature makes their interfacial processes highly responsive and metastable.

To probe these complex interfacial dynamics beyond the limits of conventional microscopy or invasive electron/x-ray-based methods, we employ a microscale functional imaging approach, *Correlation Clustering Imaging Microscopy* (CLIM). CLIM captures photoluminescence fluctuations that reflect local defect activity and carrier recombination dynamics, thereby linking interfacial functionality directly to optoelectronic behavior. Correlative CLIM–SEM imaging of perovskite thin films reveals how structural heterogeneities manifest as spatial variations in defect-mediated emission dynamics. Strikingly, when these films are integrated into complete solar cell architectures, both the amplitude of photoluminescence fluctuations and the spatial extent of active interfacial regions increase markedly and evolve with the device's operational regime.

Through statistical analysis of intensity fluctuations, we uncover distinct metastable defect processes driving non-radiative recombination at interfaces within both thin films and working devices. These insights demonstrate how interfacial dynamics govern macroscopic efficiency and stability, establishing microscale functional imaging as a powerful route to engineer and optimize interfacial properties in next-generation optoelectronic devices.

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Sudipta Seth is currently a Marie Skłodowska-Curie Postdoctoral Fellow at KU Leuven, Belgium, where he conducts advanced research at the intersection of materials chemistry, optoelectronic devices, and photophysics, through the development of innovative microscopy methodologies. He completed his PhD at the University of Hyderabad and subsequently worked as a postdoctoral fellow at Lund University and as a visiting junior fellow at the Tokyo Institute of Technology. His work integrates single-particle spectroscopy, super-resolution and nanoscale microscopy, and ultrafast spectroscopy to investigate fundamental photophysics in semiconductor materials and devices. He has received several academic fellowships, including INSPIRE-SHE (India), Wenner-Gren Postdoctoral Fellowship (Sweden), FWO Research stay abroad (Belgium), and Marie Sklodowska-Curie Postdoctoral Fellowship (European Commission).

Decoupling Excitons from High-Frequency Vibrations in Organic Molecules

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The coupling of excitons in π-conjugated molecules to high-frequency vibrational modes (1,000–1,600 cm^{-1}) has long been viewed as unavoidable, accelerating non-radiative losses and limiting the efficiency of light-emitting diodes, biomarkers, and photovoltaics. Here we combine broadband impulsive vibrational spectroscopy, first-principles modelling, and synthetic chemistry to investigate exciton–vibration coupling across diverse π-conjugated systems. We identify two molecular design rules that decouple excitons from high-frequency vibrations. First, when the exciton wavefunction exhibits strong charge-transfer character with spatially separated electron and hole densities, high-frequency modes become localized on either donor or acceptor units, minimally perturbing the exciton energy. Second, selecting orbitals with symmetry-imposed non-bonding character effectively removes coupling to high-frequency modes that modulate π-bond order. We exemplify both rules using spin-radical systems showing efficient near-infrared emission (680–800 nm) from charge-transfer excitons, where significant coupling occurs only below 250 cm^{-1}—too low to drive rapid non-radiative decay. Consequently, non-radiative rates are suppressed by nearly two orders of magnitude relative to π-conjugated molecules of similar bandgap. These results demonstrate that losses from coupling to high-frequency vibrations are not an intrinsic limitation of organic emitters and provide a rational framework for designing low-loss molecular semiconductors.

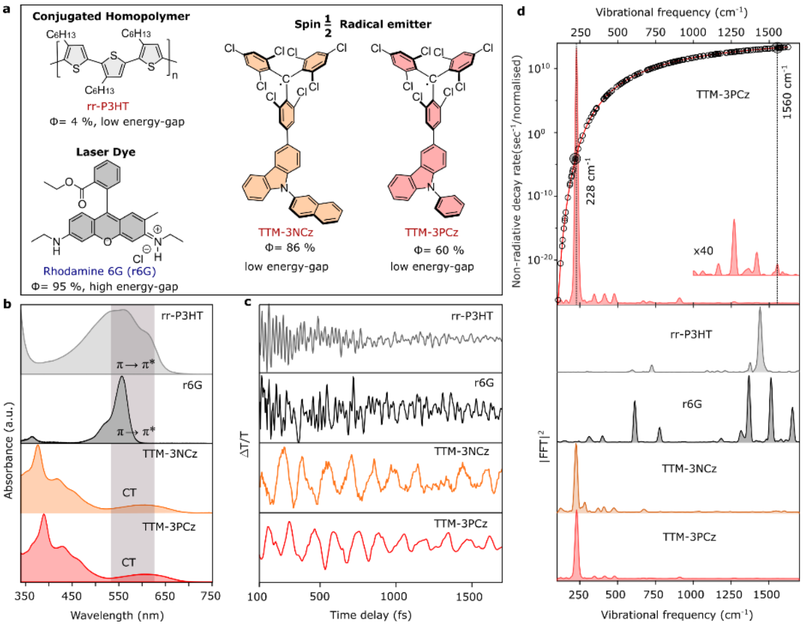

Figure 1. Vibrational decoupling in the high-frequency regime for organic optoelectronics

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Dr. Pratyush Ghosh is a Research Fellow at St John's College, University of Cambridge, where his work explores the ultrafast dynamics of photo-induced processes in condensed-phase systems. His research focuses on developing and applying time-resolved spectroscopic techniques to investigate the interplay between electronic and nuclear motion in complex molecular environments.

Before joining St John's, Dr. Ghosh completed his PhD in Chemistry at the University of Cambridge, where he studied ultrafast structural dynamics in solution using advanced transient absorption and ultrafast vibrational spectroscopies. His earlier education was at the Indian Institute of Technology Kanpur (IIT Kanpur), where he received his MSc degree in Chemical Sciences and BSc degree in St John's College, Kolkata.

Dr. Ghosh's scientific interests centre on understanding molecular photophysics and photochemistry at fundamental timescales, with broader implications for energy conversion, catalysis, and material design.

Tin vs. Lead Halide Perovskites: Interlinked Yet Distinct Colloidal Nanochemistries of Growth and Stability

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The colloidal nanochemistry of tin halide perovskites draws inspiration from their well-studied lead-based counterparts; however, owing to their intrinsic instability and complex reactivity, it remains far less understood and controlled. Despite these challenges, their reduced toxicity and promising optoelectronic properties underscore the importance of understanding their chemistry to achieve stable, high-performance materials. In my talk, I will discuss how, despite their structural similarity, the nanochemistry of tin and lead halide perovskites diverges significantly, influencing their dimensional dynamics,[1] growth pathways, and nanostructural integrity.[2,3] Using $FASnI_3$ (FA: formamidinium) as a representative system, we highlight the critical influence of ligand binding on the formation and dimensionality of tin halide perovskite nanostructures. Even trace amounts of long-chain ammonium ligands such as oleylammonium induce the emergence of mixed 2D–3D architectures, emphasizing the sensitivity of tin-based systems to amine coordination. This observation motivated us to develop an amine-free, three-precursor synthetic route, which enables controlled growth of phase-pure 3D $FASnI_3$ nanocrystals. Furthermore, the factors that govern and facilitate heterogeneous overgrowth on existing perovskite nanostructures were examined *via in situ* studies of nanocrystal growth kinetics.[4] Overall, these insights establish guiding principles to achieve precise control over perovskite nanochemistry, paving the way for sustainable perovskite optoelectronics.

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Kushagra Gahlot is a Humboldt post-doctoral fellow at the Chair of Photonics and Optoelectronics in Nano-institute, Ludwig Maximilian University of Munich, Germany. His research focuses on the nanochemistry, surface engineering, and photophysics of sustainable semiconductor materials.

He received his bachelors in chemistry from Hindu college, University of Delhi in 2012. He then completed his M.S. in chemical sciences at Jawaharlal Nehru Center for Advanced Scientific Research (JNCASR), Bengaluru, where he investigated transition metal doping of II-VI semiconductor nanocrystals. Subsequently, he was awarded a top master's nanoscience scholarship to pursue a highly interdisciplinary master programme at the Zernike Institute for Advanced Materials, University of Groningen, The Netherlands, and pursued a project on the fabrication and characterization of tin halide perovskite based solar cells. For his Ph.D., he joined the research group of Prof. Loredana Protesescu in the same institute, and extensively worked on understanding and developing the colloidal nanochemistry of tin-halide perovskites. In 2024, he successfully defended his Ph.D. thesis titled "Tin Halide Perovskite Nanostructures".

He received recognition as a best poster prize winner (Next-Gen Photovoltaics Conference 2024 and Zernike Ph.D. Colloquium 2022) and a CeNS travel awardee 2024. He served as a student member of the programme committee for nanoscience (2017-2019) and as a sounding board member to the Graduate School of Science and Engineering (GSSE), University of Groningen (2020-2023). Currently, he is organizing the Gordon Research Seminar (GRS) on "Colloidal Semiconductor Nanocrystals 2026" as an elected co-chair.

Poster Presentation

Fluorescence Tuning in DADQ-Based Materials: Dielectric and Chiral Environment Effects

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Molecular solids exhibiting enhanced fluorescence in the aggregate/solid states are stimuli-responsive materials holding great promise for optoelectronic[1] and sensing applications.[2] Fluorescence response tuning can be achieved by molecular design or controlling supramolecular assemblies. We have demonstrated the fine-tuning of the fluorescence emission of diaminodicyanoquinodimethane (DADQ) based molecules, on brief exposure to acetic acid vapors, inducing weak protonation and subtle changes in the dielectric environment of the fluorophore.[3] Spectroscopic studies confirm the protonation effect; computational modelling of the electronic states of the DADQ molecule incorporating standard solvation models, together with experimental verification using impedance spectroscopy and surface potential measurements, generalizes the concept. We have also demonstrated enhanced sensitivity of a chiral DADQ derivative towards enantioselective recognition. The (*R*,*R*) and (*S*,*S*) enantiomers interact with (*D*) and (*L*)-mandelic acid, with an enantioselectivity factor (***ef***) of the order 1-3, at μM analyte concentrations. We have developed a novel approach to amplify the enantioselectivity using diastereomeric complexes of the chiral fluorophore on a chiral substrate; in the present example, the ***ef*** could be enhanced to ~ 25 - 50 using complexes of the chiral fluorophore adsorbed on nanocellulose.[4] The amplification of enantioselectivity using the adsorbate-adsorbent complexes is shown to be a general effect, as illustrated with a selection of other chiral analytes.

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Triazenyl Radical: A New Class of n-Type Dopant

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Organic semiconductors, pioneers of flexible and bendable electronics with lower conductivity than their inorganic counterparts, require doping to fabricate real-world devices. However, n-type dopant development has lagged behind p-type doping due to instability issues and the inefficient doping capability of the current class of dopants. My work focuses on the development of a new class of n-type dopants based on organic free radicals, which are capable of doping some well-known n-type semiconductors.

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N-type Conducting Polymer with The Highest Conductivity

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Transparent conductors are essential for devices such as LEDs, solar cells, electrochromic systems and touch screens. Although ITO offers high transmittance (80–85%) and low sheet resistance (~15 Ω/sq), its high cost and brittleness limit use in flexible processing. Existing n-type organic semiconductors are not suitable as transparent conductors due to low conductivity, poor optical transparency and instability. Recently, n-doped PBFDO has emerged as a stable, high-performance n-type organic conductor; however, its synthesis is time-consuming, requiring several days of dialysis or metal incorporation. In this work, we introduce a fast (<1 hour), one-pot synthesis that is completely metal-free and purification-free, while being scalable, ambient-stable and solution-processable. This approach offers a cost-effective alternative to conventional metal inks and transparent electrodes for next-generation display and solar technologies.

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Effect of Thiophene-Sulfoxide and Dimethyl Sulfoxide on Lipid Bilayer Porosity

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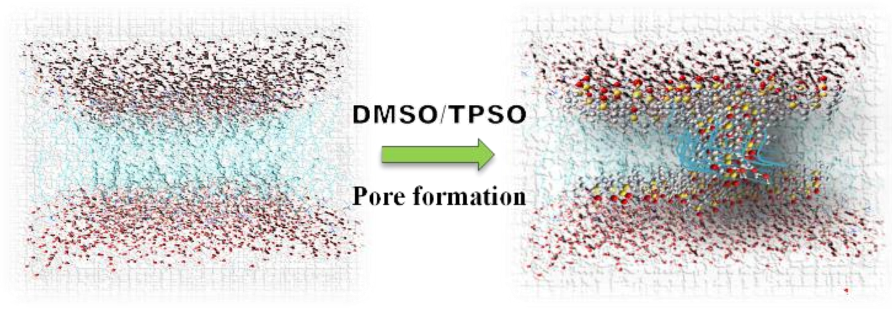

Interactions between small amphiphilic solvents and lipid bilayers play a central role in modulating membrane structure, dynamics, and permeability. In this study, we examine how dimethyl sulfoxide (DMSO) and thiophene-sulfoxide (TPSO) influence bilayer organisation using the photophysical responses of embedded fluorescent probes, coumarin and Rhodamine 6G (Rh6G). Coumarin, which is highly sensitive to microenvironmental changes, exhibited more pronounced spectral shifts in TPSO-modified bilayers than in those containing DMSO, suggesting stronger perturbation of bilayer structure. Time-resolved fluorescence measurements showed reduced lifetimes in both solvent-modified systems relative to native bilayers, consistent with increased membrane porosity or enhanced molecular motion. FRET analysis further revealed shorter donor–acceptor distances and higher transfer efficiencies in TPSO-containing bilayers, indicating tighter spatial confinement of probes and altered membrane packing. Collectively, these results demonstrate that TPSO induces more substantial reorganisation of lipid bilayers than DMSO, enhancing molecular mobility and energy-transfer processes. The mechanistic insights gained here establish TPSO as a promising tool for probing membrane dynamics and for applications in fluorescence-based sensing and drug-delivery strategies.

Unusual Fluorescence Behaviour of Different Dyes: A Study in Protonated and Deuterated Solvents

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This study investigates how solvent environments influence the photophysical behaviour of three organic dyes with distinct charge characteristics: Rhodamine 6G (positive), Fluorescein salt (negative), and Phenyl anthracene (neutral). Steady-state absorption and fluorescence emission spectra were recorded in protonated and deuterated solvents, including H_2O, D_2O, CH_3OH, CD_3OD, $(CH_3)_2SO$, and $(CD_3)_2SO$, followed by time-resolved fluorescence lifetime measurements. The results demonstrate that dye emission behaviour is governed not only by solvent viscosity but also by hydrogen-bonding interactions and associated isotopic substitution effects. Excited state energy dissipation through hydrogen bonding is more efficient in protonated environments than in their deuterated counterparts for negatively charged dyes (fluorescein disodium salt), whereas for positive one (rhodamine 6g), energy dissipation are same. Negatively charged dyes release it's excited state energy through hydrogen-bonded protons more than deuterated ones. In case of positively charged dyes, the solvent cage is formed by keeping the "O" atom towards the inner side, wherein the protons /deuteriums are remaining towards the outer side. So, the excited state energy dissipation for positively charged dyes is the same as the environment for protonated solvents and deutriated solvents are the same. Similarly, for neutral molecules like phenyl anthracene releases its excited state energy more in a protonated solvent than a deuterated one only because of random interaction with proton/deuterium as well as "O" atom. Overall, this work clarifies how dye–solvent interactions govern excited-state behaviour, enabling more informed design of fluorescence probes and sensing systems.

Photocatalytic Oxidation of Organic Sulfides inside Water-soluble Nanocages

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Aromatic sulfoxides are very important building blocks for the synthesis of fragrances, and pharmaceutical ingredients[1]. Traditionally the synthesis of sulfoxides generally requires stoichiometric use of oxidizing agents (H_2O_2), metal oxides, and photosensitizers[2]. Although they give moderate to good yield in reaction turnovers but the often associated with the formation of toxic sulfone as side product and use of transition metal-based catalyst and organic solvent generate toxic wastes. To address these challenges and to synthesize aromatic sulfoxides, we have chosen to synthesize a supramolecular cage with a capping ligand. We focused into utilizing the donor-acceptor CT interactions formed between electron-rich aromatic sulfide molecules and electron-deficient cavities. The cavity synthesis was done in three steps as per the literature protocol[3]. We optimized the reaction condition for various substrates with cationic nanocage and after optimization of the photocatalytic reactions, we found the selectivity of sulfoxide products going up to 100 % from GCMS. We probed the formation of radical cations on the sulfides[4] and anion radicals on the triazine panel[5] from transient absorption measurements and low-temperature EPR spectroscopy enabled the detection of a cage-confined sulfide radical cation–O_2 adduct, suggesting a single electron transfer event.

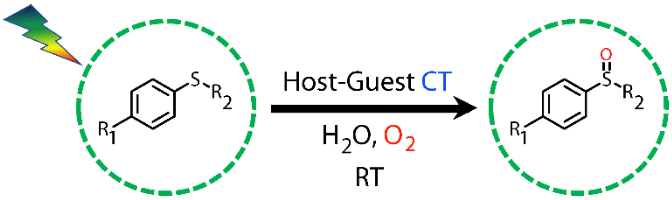

Figure 1. Conceptual representation of visible light-mediated sulfide oxidation inside cationic $Pd_6L_4^{12+}$ nanocage.

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Smart Multifunctional Polymersome Nanocarrier for Broad-Spectrum Biofilm Eradication and Accelerated Healing of Infected Wounds

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Antimicrobial resistance (AMR) has become a defining biomedical challenge, undermining existing antibiotics and accelerating the spread of multidrug-resistant pathogens.[1-2] Alongside bacterial genetic adaptability, physicochemical defense strategies—such as biofilm formation, intracellular persistence, metabolic dormancy, and reduced membrane permeability—further limit antibiotic penetration and promote chronic, treatment-refractory infections. Biofilm-associated infections, in particular, exhibit strong tolerance to conventional therapeutics and contribute to delayed tissue repair and persistent inflammation.[3]

Here, we present crosslinked cationic polymersomes as smart nanotherapeutics engineered to address both biofilms and impaired wound healing. The polymersomes feature a stable crosslinked membrane and tunable cationic surface, enabling strong interactions with negatively charged biofilm matrices and deep penetration into mature biofilms. This architecture accelerates disruption of the EPS network, enhances bacterial killing, and sustains antimicrobial activity under physiological conditions.

In vitro, the nanocarriers display potent inhibitory effects against polymicrobial biofilms formed by Gram-positive and Gram-negative bacteria. In vivo infected-wound studies show rapid re-epithelialization, reduced bacterial load, and attenuated inflammatory cytokines, demonstrating the dual antibacterial and wound-regenerative functions of the system.

Collectively, this multifunctional polymersome platform offers a promising therapeutic strategy for combating biofilm-driven infections while promoting effective wound repair, addressing critical unmet needs in next-generation anti-infective nanomedicine.

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Luminescent Organic Single Crystals as Multi-Output Channel and Flexible Optical Waveguides for Visible Light Transmission

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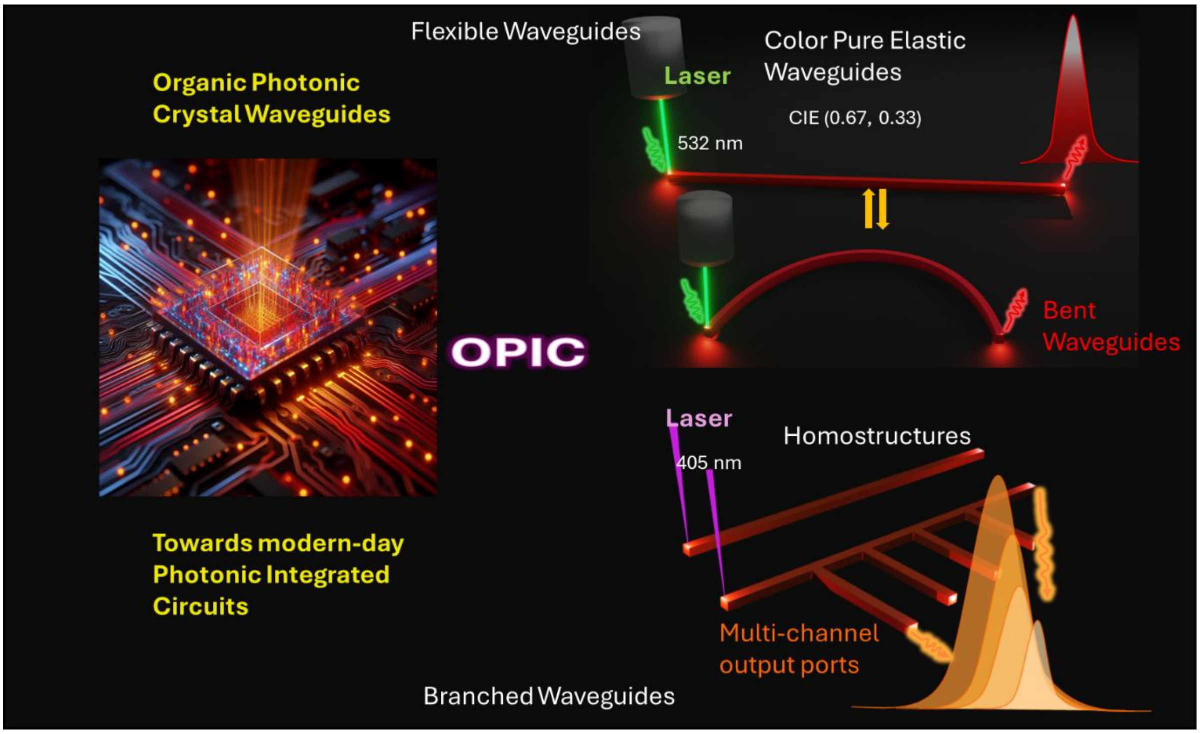
Organic crystalline materials have emerged as an essential class of solid-state materials in the field of nanophotonics. Mechanically soft luminescent crystals actively contribute towards the design of optical waveguides (OWGs) with high optical performance for fabricating next-generation telecommunication and integrated photonic devices. Herein, we achieved the design of two Schiff base compounds with active waveguiding properties, with one exhibiting excellent elastic flexibility along with the rare property of pure red emission with the standard Commission Internationale de l'Eclairage (CIE) coordinates of (0.67, 0.33).[1] On the contrary, self-assembled branched homostructures of another model compound demonstrated multi-input/output optical-waveguiding behavior,[2] expanding the potential of such materials in integrated photonic circuits. Such multiple output optical components with various light-waveguide channels offers the possibility for meeting the requirements for multifunctional optical circuits in modern-day photonic devices.



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Thermal and Photoswitching Luminescent Organic Molecules for Information Encryption-Decryption

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Chromic materials have garnered much attention due to their reversible color change under various stimuli such as light, heat, pH, pressure, electric current, etc., making them an excellent choice for photoswitches, anti-counterfeiting devices, rewritable inks, temperature sensors, etc.[1,2]

Herein, we designed a schiff base, exhibiting synergistic photochromic and thermochromic response which reversibly alters its absorbance and emission properties with stimuli. Systematic studies were done to analyse the spectroscopic and structural changes associated with these responses in the molecule. The reversible and fatigue-resistant thermochromic and photochromic responses under heat and UV-visible light respectively has been extensively utilised in rewritable inks and information encryption-decryption. This work further expands the scope of stimuli-responsive chromic luminescent organic materials for modern-day smart applications.

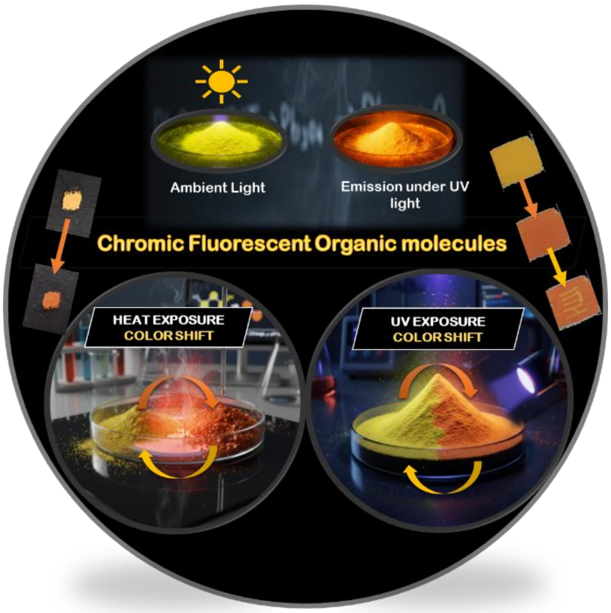

Fig.1. Graphical illustration showing photo and thermal response shown by the as prepared compound.

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Halogen-Mediated Non-Covalent Interactions Induced Anomalous Fluorescence Shift in Crystal: Temperature Sensor from 20K to 370K

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Organic luminescent crystals are getting enormous attention as external stimuli responsive smart materials.[1,2] Herein, we introduce three naphthol-based fluorophore crystals having specific halogen-mediated non-covalent interactions (NCI), because of the presence of two halogen atoms in the attached phenyl ring. As we go from –Br to –Cl to –F, unlike the literature reports,[3] bathochromic-shift of the fluorescence maximum has been observed.

Temperature is one of the most measurable external stimulus thermodynamic parameters. The luminescent materials can detect temperature with the changes of (i) emission intensity, (ii) emission maximum, (iii) ratiometric emission intensity, and (iv) excited-state-lifetime.[4–6] Out of them, first three are based on steady-state, whereas (iv) requires expensive time resolved spectrofluorometer. Among others the sensitivity of (ii) and (iii) are much better and hence these methods are highly sought after phenomena for sensitive temperature sensing. Although, there are very few literature reports of temperature sensing employing organic crystals,[4–6] however there is no literature report for below 80K.

Interestingly, among them, F-substituted one can accurately sense temperature from 20K to 370K, employing temperature dependent (a) shift of emission maximum, and (b) ratiometric emission intensity. Halogen-mediated NCI have been found to be the major reasons responsible for the above-mentioned interesting observations.

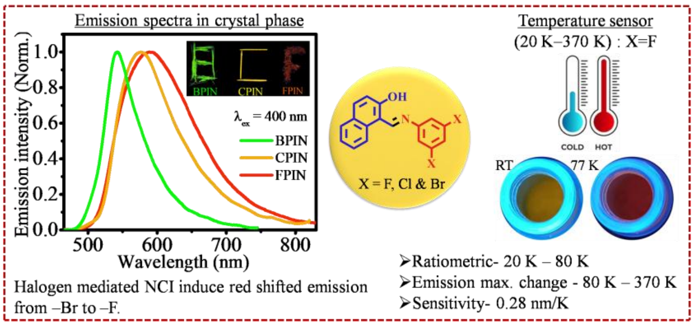

Figure 1. Schematic diagram.

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Exploring the Potential of Meta-oriented Donor-Acceptor Organic Systems in Efficient Room-Temperature Phosphorescence

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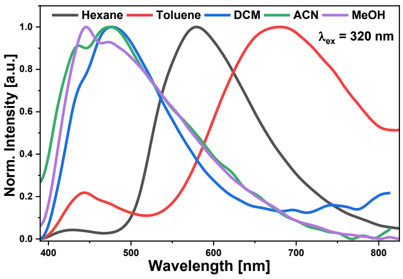
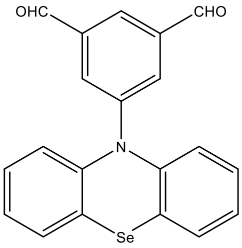
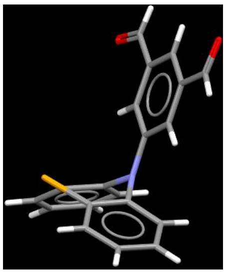
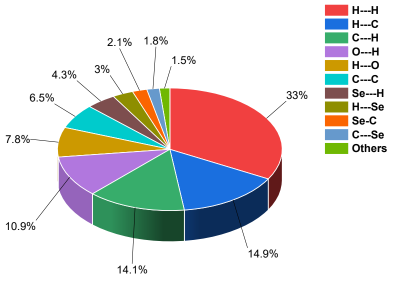
Room-temperature phosphorescence (RTP) is a phenomenon characterized by long-lasting light emission resulting from the radiative decay of triplet excited states.[1] The tunable electronic properties of donor-acceptor (D-A) organic systems enable precise control over photophysical behavior, making them highly suitable for designing RTP materials.[2] Traditionally, chemists have focused on ortho and para configurations of D-A systems due to their intramolecular charge transfer (ICT) characteristics. However, recent findings demonstrate that meta-oriented D-A systems also exhibit excellent ICT capabilities, distinguished by low molecular weight, high quantum yield, large Stokes shift, prolonged excited-state lifetime, and red-shifted emission.[3]

In this study, we synthesized and characterized a D-A molecule named **SeDiCHO**, which incorporates a phenoselenazine donor unit and two formyl acceptors attached to a benzene ring in a meta configuration. Photophysical analysis in solution revealed two different conformations attributed to the phenoselenazine group.[4] Conversely, photophysical studies combined with single-crystal X-ray diffraction confirmed an axial conformation within the crystal lattice. Notably, SeDiCHO demonstrated phosphorescence at approximately 560 nm with a lifetime of 7 milliseconds in the crystalline state. Computational modeling and experimental data suggest that Vanderwaal interactions stabilize the crystal structure and facilitate the formation of the triplet excited state, which is responsible for the observed phosphorescence.









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Visible-Blind HTL-Free UV-C Photodetector Based on Ruddlesden-Popper (RP) Pure 2D PEA_2PbBr_4 Perovskite Thin Film

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The development of efficient and stable ultraviolet photodetectors, particularly those sensitive to the UV-C spectrum (200-280 nm), is crucial for diverse applications including environmental monitoring, sterile medical systems, and secure communication. Traditional wide-bandgap semiconductors from II-VI compound semiconductors have been extensively utilized for such applications; however, their fabrication often involves high temperatures and complex processes. In contrast, metal-halide perovskites have emerged as promising alternatives due to their low-cost processing, high absorption coefficient, tuneable optoelectronic characteristics and long charge carrier diffusion length of these materials make them highly attractive for next-generation photodetector technologies.[1–3] Herein, we present a solution-processed, high-performance, visible-blind, hole-transport-layer-free UV-C photodetector leveraging a pure 2D PEA_2PbBr_4 thin film, achieving a responsivity of 0.4 mA/W and a detectivity of 1.2×10^9 Jones. The rise and fall time of the fabricated devise is found to be 27 μs and 24 μs respectively which is superfast and makes us believe that the availability of such devices may pave the way for ultrafast optical communications and other optoelectronics systems which are specifically used in indoor or visible light conditions.

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Solution-Phase Molecular Dynamics: Linking Aggregation and Chirality Through Optical and Electrical Signatures

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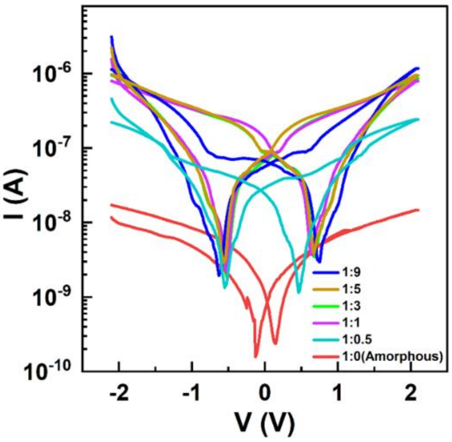
Molecular assemblies in solution offer a powerful framework for understanding how subtle changes at the nanoscale translate into large variations in optical and electronic behavior. In this work, we track the evolution of π-conjugated systems as they move through distinct aggregation regimes, beginning with primary nucleation from molecularly dispersed states and eventually reaching surface-assisted secondary nucleation that produces extended 2D sheets and dendritic architectures. These progressive structural transformations reshape the effective electronic landscape and give rise to clear, quantifiable changes in device measurements, including enhanced conductivity, reduced hysteresis, and noticeable increases in maximum channel current as packing becomes more ordered and π–π pathways strengthen. When the aggregation processes produce chiral, helical domains, we also observe the emergence of strong circular dichroism together with measurable differences in photocurrent under left- and right-circularly polarized illumination. The chirality of the assemblies can be followed by tracking the g-factor associated with the photocurrent; we obtain values in the range of 0.55–0.61, which are among the highest reported for solution-phase supramolecular semiconductors. This tight correlation between supramolecular growth and chiroptical response enables a real-time electrical readout of evolving chirality directly from the solution.



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Exploring Organic FeFETs with Novel Ferroelectric Layers: A Route Toward Efficient In-Memory Neuromorphic Computing

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Neuromorphic computing architectures that mimic brain-like information processing offer significant advantages for energy-efficient artificial intelligence and in-memory computing. This work investigates the neuromorphic performance of organic FEFETs fabricated using novel solution-processable ferroelectric materials based on metals. Electrical characterization demonstrates stable ferroelectric switching with well-defined memory windows. Neuromorphic measurements reveal long-term potentiation/depression (LTP-LTD), spike-timing dependent plasticity (STDP), and paired-pulse facilitation/depression (PPF-PPD), confirming synaptic emulation capabilities. Memory retention and endurance testing show device longevity, while performing suitable handwritten pattern recognition.

These insights will directly contribute to advancing neuromorphic device technology and accelerating the development of energy-efficient in-memory computing systems that can overcome the limitations of conventional von Neumann architectures.

Keywords: Ferroelectric materials, organic field-effect transistors, neuromorphic devices, solution processing, synaptic plasticity

High-Entropy Halide Perovskites for Opto-Electronic Devices

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Halide perovskites are promising for next-generation optoelectronic materials due to their variable bandgaps, high absorption coefficients, long carrier diffusion length, and better charge transport abilities. However, low environmental stability and lead (Pb) toxicity, which creates major environmental and health problems, severely limits their applications in solar cells, LEDs, and photodetectors in large scale manufacturing. As an alternative, high-entropy halide perovskites (HEHPs) can stabilize the crystal lattice and reduce the amount of Pb without hindering the performance of optoelectronic devices. This is achieved via the addition of multiple cations to one crystallographic site by increasing configurational entropy. In contrast, single-crystal perovskites are also able to reduce flaws at grain boundaries, reduce trap states, and make devices more efficient and stable. This work developed stable HEHPs materials that are potentially suitable for both LEEC and LED devices, featuring reduced Pb content without sacrificing opto-electrical performance.

Keywords: HEHPs, LEEC, LED, Single-crystal

Correlation of Morphology & Interface Properties with Charge Transport in Wide Band Gap Perovskite Solar Cells

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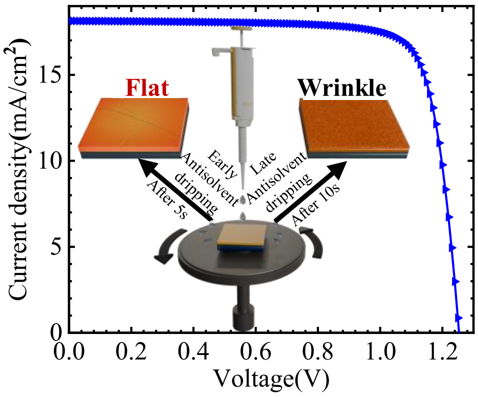
Wide band gap (WBG, E_g~1.8 eV) perovskite solar cells (PSCs) is a key element for all-perovskite tandem solar cell technology. Here, we investigate the effect of morphology on charge transport properties in PSCs with ~1.8 eV absorbers. Morphologies are tuned via anti-solvent dripping timings. Early dripping produces flat films with cracks, while delayed dripping results in wrinkled morphology. Temperature-dependent photoluminescence measurements reveal that wrinkled films exhibit lower activation energy, indicating improved charge transport. Further, scanning photocurrent microscopy reveals that wrinkled films possess significantly higher lateral charge transport lengths (L) for photo induced charge carriers as compared to flat films, and a further improvement in L is achieved through interface passivation. This morphology-driven enhancement, along with interfacial engineering, reduces non-radiative voltage losses, yielding a power conversion efficiency of 18.26%. Overall, this study establishes a direct correlation between morphology-induced enhancements in charge transport and minimized voltage losses in WBG PSCs.



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Laser Guided Micro-Bubble Lithography (MBL) Printed Electrodes for The Water Energy Nexus

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Microbubble-based lithographic techniques have rapidly evolved as a versatile platform for precision patterning of multifunctional materials, enabling the development of advanced microelectrodes and electrocatalytic devices. Building on this foundation, two distinct studies highlight the transformative impact of microbubble lithography (MBL) in energy materials engineering. The first demonstrates the instantaneous in-situ synthesis and micro-patterning of ZIF-67, a zeolitic imidazolate framework (MOF), via MBL, yielding stable microelectrodes for the oxygen evolution reaction (OER) and establishing a pathway for integration into lab-on-a-chip systems for diverse catalytic applications. Complementing this, the second work introduces a template-free MBL approach for fabricating highly ordered $Zn_{10}In_2S_{13}$ (ZIS) nanostructures, achieving bifunctional activity for both OER and the selective $4e^-$ oxygen reduction reaction (ORR) critical for metal–air batteries. Both studies exemplify how microbubble-induced nanoarchitecture engineering affords controlled exposure of active sites and tailored electronic properties, driving selective and durable electrocatalysis. The convergence of MBL-enabled microfabrication and catalytic material design paves the way for next-generation energy conversion devices and miniaturized electrochemical platforms.

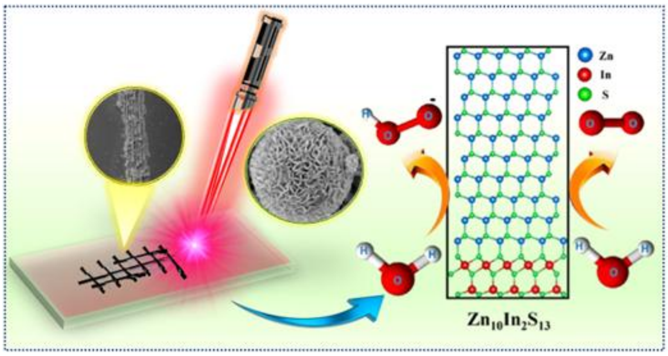

Figure 1. Schematic of Laser Guided Micro-Bubble Lithography (MBL) Printed Electrodes for the Water Energy Nexus.

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Additive Free Formation of Aldol and Polyacetone from Acetone Under Pressure

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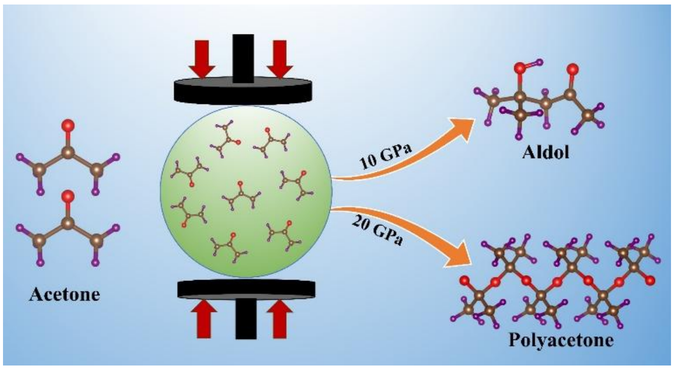
Pressure induced polymerization (PIP) provides a route towards the controlled synthesis of topological polymeric compounds from the basic molecular units. In general, PIP is a green chemical process without the requirement of solvents, additives or catalysts. Siloxane, a backbone polymer containing alternating silicon and oxygen linkage with organic side chains are commercially known as silicone oil. Herein we report a new class of polymeric compound formed by molecular acetone using crystal structure predictions assisted by first-principles calculations at high pressure ($P \geq 20$ GPa). Acetone forms a polymeric compound with alternating carbon − oxygen linkage, $[-(Me)_2C-O-C(Me)_2-]_n$ analogous to the polydimethylsiloxane (PDMS) structures. This polymeric structure is dynamically stable over wide range of pressures and thermally stable at room temperature. The present finding establishes the first-example of carbon based PDMS type-structure and should motivate further exploration in novel polymerization protocols. At an intermediate pressure P=10 GPa, acetone self-dimerizes into the aldol (diacetone alcohol, DAA). While aldol formation from acetone traditionally requires external acid or base catalysts, pressure in itself suffices for this reaction. The self-dimerization of acetone occurs via a hydrogen-bonded keto-enol co-crystal formed in-situ under pressure.



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Interplay of Dynamic Defects and Ultrafast Carrier Dynamics in Lead Free Double Perovskites Toward Stable, High-Performance Photovoltaics

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Oxide-based double perovskites are gaining increasing attention as stable and environmentally benign alternatives to halide perovskites in photovoltaic and optoelectronic devices. Their structural versatility and chemical flexibility open pathways for fine-tuning both electronic and lattice properties, yet their carrier dynamics and defect behavior remain less understood. In this work, we investigate these aspects using a combination of first-principles calculations and advanced simulation techniques.

Nonadiabatic molecular dynamics is employed to capture ultrafast carrier relaxation and to quantify the role of electron–phonon coupling in determining charge transport and recombination lifetimes. The results highlight efficient charge separation and suppressed nonradiative recombination channels, which are essential for high photovoltaic efficiency. To establish the dynamical stability of the materials, we carry out a phonon-based symmetry analysis that confirms the absence of imaginary modes and reveals the interplay between structural distortions and vibrational spectra. In parallel, we explore the formation and dynamic evolution of intrinsic point defects through defect-mediated molecular dynamics simulations. These studies shed light on migration pathways, possible defect-assisted recombination channels, and their impact on overall carrier dynamics. The comparative analysis reveals how compositional variations influence defect tolerance, lattice anharmonicity, and the balance between radiative and nonradiative processes.

Together, these insights provide a comprehensive understanding of the interplay between electronic excitations, lattice vibrations, and defect physics in oxide-based double perovskites. The findings point toward design strategies for engineering defect-resilient, dynamically stable photovoltaic absorbers with long carrier lifetimes, thereby advancing the development of robust next-generation solar materials.

Routes to Improve The Photoluminescence Efficiency in Low-Dimensional Halide Perovskites

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While the resurgence of interest in hybrid halide perovskites began with the possibility of using them as active components of solar cell materials, very soon they were found to exhibit superior optoelectronic properties. In this talk I will present some recent work using density functional theory based calculations on routes to achieve high photoluminescence quantum yield (PLQY) in a class of low dimensional halides in which the presence of defects is inevitable. We have calculated the formation energies and identified the dominant source of defects. These correspond to halide vacancies and introduce states within the band gap region. The presence of these states promotes nonradiative recombination pathways, thereby suppressing radiative transitions and hence reducing PLQY. These defect states can be effectively mitigated through targeted doping, which then helps in suppressing defect-mediated carrier trapping, and hence enhancing radiative recombination. The design principles involved in this approach will be presented considering the case of $Cs_2InBr_5.H_2O$.

Organic Scaffolds for Tunable Triplet Emission: A Computational Perspective

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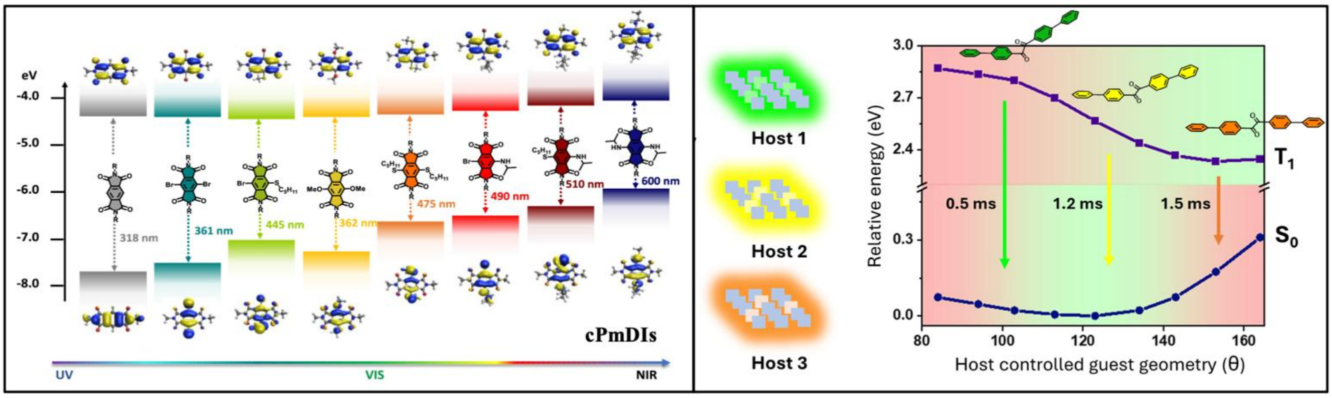
The pursuit of cost-effective, non-toxic, and highly efficient organic chromophores remains critically important for their application in optoelectronic devices. Pyromellitic diimides (PmDIs), a class of n-type arylene diimide semiconductors, serve as a versatile scaffold for engineering tunable triplet emission. Core substitution strategy to PmDIs not only induces a wide spectrum of fluorescent colors, but enables a wide-range of phosphorescence spanning across visible spectra. In this context, we have performed calculations on various core-substituted PmDIs. Using first-principles theory, we have elucidated the underlying mechanism by which core substitution enables precise modulation of triplet-state emission, spanning a range of 190 nm across the visible spectrum. Notably, thio-substitution leads to simultaneous ambient phosphorescence as well as TADF emissions.[1]

Theoretical investigations on a class of organic host-guest systems reveal that the photoexcited conformational dynamics of guest molecule diphenylbenzil (DPB) is responsible for RTP color variation. Trace amounts of DPB in various organic matrices (host) ensued tunable RTP color from green to orange-red. Furthermore, in an appropriate host matrix, a linear conformer of guest DPB was stabilized, resulting in improved quantum yield. This work presents a novel trace doping strategy for developing RTP materials with tunable optical features by synergistically controlling the ground and excited-state geometries of a single molecule.[2]



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Computational Insights into Molecular Engineering of Small Molecule Electron Donors Towards High-Efficiency Organic Solar Cells

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Organic Solar Cells (OSCs) have emerged as a promising pathway towards a clean energy future. Accelerated research interest over the last few decades has led to remarkable breakthroughs in the development of next-generation photovoltaic technologies. However, wide-scale industrialization of OSCs requires further improvement in PCE and device stability under in-field operating conditions.[1] This can be achieved through the effective screening of various light-harvesting organic materials, which facilitates easier synthesis of the active layer and enhances solar energy absorption and exciton dissociation at the D/A interface, thereby enhancing the power conversion efficiency (PCE). Hence, in our work, we have investigated novel small molecule electron donors (SMDs) employing diphenylamine (DPA) and naphthobisthiadiazole (NTz) based units. Density Functional Theory (DFT) and Time-Dependent DFT (TD-DFT) methodologies have been employed to investigate the solar energy harvesting and charge generation capabilities of the designed systems.[2] Our findings, comprising the structural, electronic and optical properties, reveal that an alternating arrangement of DPA and NTz units with rational molecular engineering of the functional groups can effectively tune the optoelectronic characteristics, thereby influencing the overall PCE of an OSC. Our investigation provides a comprehensive theoretical understanding of the structure-property-performance relationship in SMDs for high-performance OSCs.

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Quantum Dot-Sensitized Photon Upconversion for Visible-Light Photocatalysis

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Visible-light photocatalysis has been established as a sustainable strategy for chemical transformations. But it operates within the thermodynamic limit set by the maximum energy of visible-light photons. This limits the range of redox potentials accessible through common visible-light active photocatalysts. Therefore, it becomes important to develop novel methodologies that can drive thermodynamically challenging reactions using visible-light. Photon upconversion based on triplet-triplet annihilation (TTA) is one such promising strategy which can convert two lower energy photons to a higher energy photon using an appropriate photosensitizer and annihilator. Upon photoexcitation, the sensitizer transfers its excitation energy to low lying triplet states of the annihilator. Two such triplet excited annihilator molecules can undergo TTA, generating one higher energy singlet excited state. This singlet state formed from the combined energy of two photons can then be utilized for photoredox catalysis.[1] Various photosensitizers have been explored for this purpose with quantum dots (QDs) being the latest candidates. They offer distinct advantages in terms of their strong and tuneable opto-electronic properties and minimal energy loss due to inter-system crossing.[2] In the present study, we have developed a QD-sensitized TTA upconversion (TTA-UC) system for performing a challenging chemical reaction. We have used the environmentally friendly indium phosphide (InP) based quantum dots as sensitizers for a green to blue TTA-UC to carry out a challenging dehalogenation reaction.[3]

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Microscopic Investigations of Spectral Instability in Mixed Halide Perovskite Microcrystals

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Metal halide perovskites are promising photovoltaic materials due to their high power conversion efficiencies, with perovskite–silicon tandem cells recently exceeding 32% efficiency.[1] Despite this progress, long-term operational instability remains a major challenge. Mixed-halide perovskites, commonly used to tune the bandgap for tandems, are particularly vulnerable to photo-induced halide segregation,[2] where illumination drives the formation of iodide- and bromide-rich domains, compromising spectral and device stability.

Most mechanistic studies have focused on thin films, while nanocrystal work has revealed illumination-induced iodine loss.[3,4] However, the mesoscale—lying between thin films and nanocrystals—remains largely unexplored. In this study, we examine the photo-induced spectral responses of individual methylammonium lead halide perovskite microcrystals (MCs) with dimensions of a few microns. We find that these MCs undergo an initial halide phase segregation, followed by irreversible iodine sublimation under continued illumination. This two-step degradation pathway highlights how ion migration and compositional instability manifest at the single-particle level. These insights provide important guidance for designing more stable perovskite materials and improving the long-term reliability of next-generation optoelectronic devices.

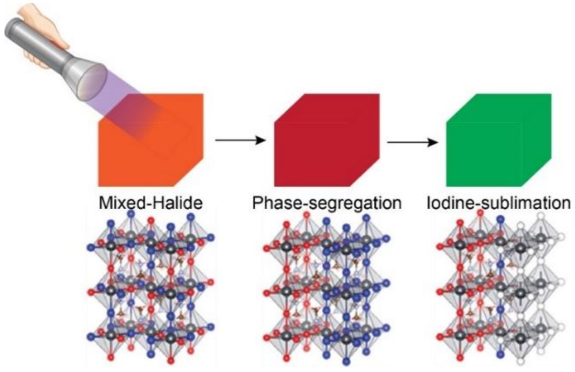

Figure 1. Phase segregation followed by iodine sublimation in mixed-halide perovskite MCs.

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Fluorescence Efficient Silver Quantum Dots with Organic Scaffold for Nucleus Imaging and Useful for Cancer Diagnosis

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Silver quantum dot synthesis by using flavanone is the challenging process. Polyhydroxy group containing flavanone, enriched with aromatic pi-electron cloud, play the role as a reducing agent and stabilizing agent for silver quantum dot synthesis. By the tuning of pH, two different sized strongly stable nanostructures are produced. Spherically shaped particles with average size of smaller particle are 2.9 nm and larger 3.5 nm. Smaller particle shows blue fluorescence (emission maxima at 410 nm) with lifetime 3.5 ns and larger particle show green fluorescence (emission maxima at 532 nm) with 2.37 ns lifetime by excitation on UV wavelength. Earlier investigation reported that thiol, amine, protein are required to synthesize fluorescent nanostructures[1] but these novel particles are synthesized without using such type of groups. Both nanostructures show strong capability to accumulate in the nucleus of the cancer cells. On incubation of cancer cells with blue or green fluorescent nanostructures, shows blue or green emission of quantum dots from nucleus by excitation at 405 nm under confocal fluorescence imaging. So these quantum dots nanostructures are unique and stands as an efficient probe of nucleus imaging as well as diagnosis of cancer cells.

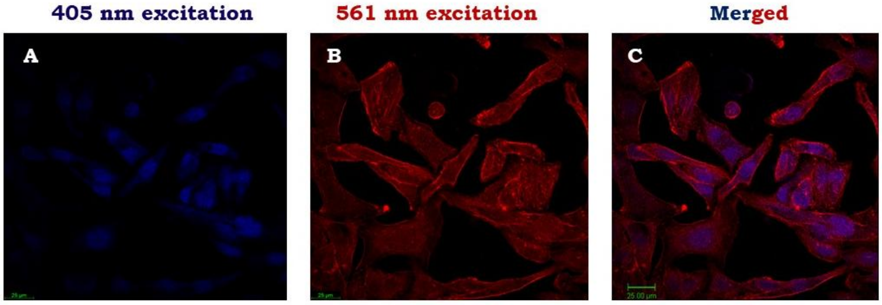

Figure 1: SKOV 3 cancer cell confocal fluorescence imaging in presence of actin binding dye (Actin Red) with blue fluorescent quantum dots. On excitation at 405 nm show blue fluorescence of quantum dots from nucleus (Fig A), on excitation at 561 nm reddish orange fluorescence from cytoskeleton (Fig B) and the merged image (Fig C). Based on these images the quantum dots are accumulated in the nucleus and shows bright fluorescence.

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Electronic Structure Engineering: Advancing Metal-free Organic Catalysts for Next-Generation CO_2 Reduction to C_{2+} Products

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Designing metal-free electrocatalysts for the transformation of CO_2 to C_{2+} products, i.e., valuable fuels, presents a significant challenge. This is largely due high energy input required to overcome the structural constraints in transforming the linear configuration of CO_2 molecules to an angular one. In this context, we explored a metal-free catalyst, diazo and dithiol-based pre-catalyst for the conversion of CO_2 to C_2 and C_3 products to develop green technology for renewable energy. A Diazo-based organic bulky ligand has a low-lying π* (LUMO) and can conveniently accept an electron from the electrochemical environment on applying potential. In the reported work, we showed Diazo-based ligand as an electrocatalyst, reducing upon applying potential to a triplet diradical that acts as a nucleophile and forms an adduct with CO_2 in an aqueous medium to form formic acid. The formic acid coupled further to form acetic acid and acetone with FE 19.6 %, and 24.2 % respectively, at pH 5.5. Furthermore, we have used a dithiol-based pre-catalyst, upon reduction, converts into thiolate anion, and the dianion acts as a soft nucleophile and is easily able to donate e^- to the LUMO of CO_2, having comparable energy with the HOMO of thiolate anion, as supported by the DFT study. We reported a heterogeneous dithiol-based electrocatalyst that selectively at a potential of -0.4 V vs Ag/AgCl at pH 5.5, form thiol-CO_2 adduct and leads to the formation of formic acid, acetic acid, and acetone with FE 7.3 %, 24.9 %, and 25.7 %, respectively. In addition, propose a possible mechanism pathway by using spectroscopy techniques and a DFT study. This study presents a groundbreaking pathway for the direct conversion of carbon dioxide into C_2 and C_3 products through an innovative organo-electroactive pre-catalyst and contributes to the development of renewable and sustainable eco-friendly systems.

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Dual-Modal Cancer Therapy via 2D-MoS_2–Peptide Conjugates for Mitochondrial Targeting and Hyperthermia

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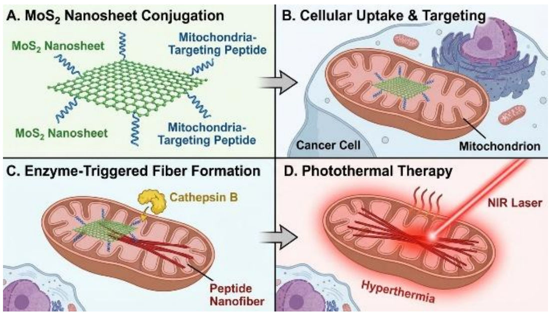
A 2D MoS_2–peptide nanocomposite was developed as a dual-mode theranostic platform that couples cathepsin B (CTB)-activated chemotherapy with near-infrared photothermal therapy for targeted cancer treatment. Defect-rich 2H-MoS_2 nanosheets were covalently functionalized with a CTB-cleavable, mitochondria-targeting peptide to afford PPCP@MoS_2 and $(PPCP)_2$@MoS_2, enabling enzyme-triggered release of a triphenylphosphonium-tagged, diphenylalanine-containing amphiphile that self-assembles into cytotoxic fibrils within mitochondria while the MoS_2 core serves as an efficient photothermal transducer.

Structural and spectroscopic analyses (XPS, PXRD, Raman, TEM/SEM/AFM, FT-IR, DLS, ζ-potential), successful peptide conjugation, nanostructure formation, enhanced luminescence, and excellent colloidal stability. CTB-mediated cleavage and peptide self-assembly were validated by TEM, HPLC, ESI-MS, and time-resolved SERS, which also enabled tracking of enzymatic responsiveness. In CTB-overexpressing HepG2 and HeLa cells, $(PPCP)_2$@MoS_2 exhibited potent chemotoxicity with negligible effects on non-malignant HEK293 cells, along with deep penetration and mitochondrial depolarisation in 2D monolayers and 3D spheroids, accompanied by ATP depletion and ROS-linked dysfunction. Under 808 nm irradiation, the construct generated robust, concentration- and power-dependent hyperthermia with excellent photothermal cycling stability, and combined chemo-PTT triggered pronounced apoptosis via caspase-9–driven intrinsic and caspase-8–assisted extrinsic pathways. This programmable, mitochondria-directed MoS_2–peptide system thus offers an all-in-one, imaging-guided platform for synergistic cancer nanotherapy.



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Conversion of 3D Lead Halide Perovskite to 2D and 1D Morphologies by Controlled Addition of Ligand-Assisted Ruthenium Complexes

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3D orthorhombic lead halide perovskite (LHP) can be converted to lower-dimensional nanostructures using various organic amine cations. Usually, both long-chain and short-chain small amine cations trigger surface exfoliation, which can lead to the formation of the 2D and 1D forms from 3D LHPs. Mixed or hetero-dimensional 3D/2D and 3D/1D perovskites are very important in photovoltaic and solar cell applications as well as in LEDs as a tool for signal up-conversion due to the improvement in surface passivation and stability. Herein, three different Ru-bipyridine [Ru(bpy)] complexes cations readily convert the 3D LHP nanocrystals into lower-dimensional nanostructures by post-treatment method. While $[Ru(bpy)_2(4,4'\text{-bpy-noyl})]^{2+}$ (RBN) generates the 2D sheet-like structures, $[Ru(bpy)_2(4,4'\text{bpy-methyl})]^{2+}$ (RBM) produced 1D rod-like morphology, which is formed through the assembling of discrete hexagonal 0D fragments. However, the third derivative, $[Ru(bpy)_3]^{2+}$, brings no change to the 3D LHPs. It is observed that the ligand molecules interact weakly with the LHP compared to the corresponding metal complex cations. It appears that RBN imposes a specific directional property to the growth of the 2D perovskite sheet due to the long carbon chain. Strikingly, replacement of the nonyl carbon chains with methyl groups leads to forming a few microns long 1D crystalline forms through the formation of 0D nanostructures. Such structural modifications in perovskites by changing the ligands in metal complex cations, and hence imposing directionality to the morphological development may serve to guiding the electron transfer dynamics in these materials.

Keywords: lead halide perovskites, metal coordination complex cations, ligands, directionality, 3D to 2D/1D conversion

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Beyond The Corona: Investigating BSA–Silver Nanocluster Interaction at Ensemble and Single-Molecule Levels

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This study explores the interaction mechanism between bovine serum albumin (BSA) and silver nanoclusters (AgNCs) to understand how proteins associate with ultrasmall nanomaterials. AgNCs were synthesized and characterized, and their interaction with BSA was systematically examined using fluorescence spectroscopy, ζ-potential, isothermal titration calorimetry (ITC), fluorescence correlation spectroscopy (FCS), and circular dichroism (CD). The fluorescence and ITC results confirm the formation of BSA–AgNC complexes, while the binding stoichiometry indicates the absence of a "protein corona," commonly observed in larger nanoparticles. FCS measurements further validate the presence of stable complexes at the single-molecule level. Thermodynamic analysis suggests that the binding is spontaneous and driven by electrostatic and hydrophobic interactions. CD spectra reveal that the secondary structure of BSA remains nearly unchanged upon complexation. Overall, the results demonstrate that BSA interacts with AgNCs through stable complex formation without significant structural alteration, providing important insights into protein–nanocluster interactions for biological applications.

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Elucidating Ligand-Controlled Charge Transfer Mechanisms in Copper Nanoclusters Through Spectroscopic Investigation

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In the recent years, nanotechnology has emerged as a fascinating branch of science dealing with the study of nano-scale sized systems. Among its many advances, atomically precise metal nanoclusters (NCs) have drawn considerable attention as atomic-level materials owing to their ultrasmall dimensions, well-defined atomic structures, abundant surface-active sites, and pronounced quantum confinement effects. These features result in discrete, molecule-like electronic structures that exhibit small-band-gap semiconductor behavior, allowing efficient light-induced excitation and generation of charge carriers (electrons and holes) that participate in photoredox processes. Despite extensive studies on various metal NCs, the exploration of photoredox reactions involving copper-based nanoclusters is still limited. Therefore, the present work focuses on elucidating the impact of surface ligands on the photophysical and electron transfer properties of Cu nanoclusters. The study examines the electron transfer interactions between two types of CuNCs and an electron acceptor, using steady-state and ultrafast time resolved studies, offering deeper insight into how surface chemistry influences charge transfer mechanisms at the nanoscale.

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Room-Temperature Polaron Dynamics in Lead-free $Cs_4CuSb_2Cl_{12}$ Layered Double Perovskite Nanocrystals

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Organic-inorganic lead halide perovskite emerged as one of the most promising materials for various optoelectronic and photovoltaic applications. As an eco-friendly alternative, a new class of lead-free double perovskite with composition $Cs_4CuSb_2Cl_{12}$ (CCSC) was reported. However, the presence of abundant surface trap states in these perovskites is the most pressing concern for commercial applications. Charge-carrier dynamics within uncapped and ligand-capped CCSC microcrystals were studied recently.[1,2] Furthermore, the effect of surface capping ligands. Oleylamine, on the physical properties and excited-state dynamics of CCSC nanocrystals (NCs) was investigated, and the results demonstrated that OAm modifies the electronic and optical properties of CCSC NCs by exclusively passivating electron trap states, thereby impacting charge carrier dynamics.[3] In this work, we explore electron-phonon coupling, which is crucial for the relaxation and mobility of the photogenerated hot carriers, It has recently been reported that spectral dispersion of a chirped continuum probe maps vibrational amplitudes as islands in the contour plot of Raman shift at different detection wavelengths, and a sum over intensities yields a spectrum of a particular vibrational mode of specific species (solute or solvent), known as broadband impulsive stimulated Raman spectroscopy (broadband ISRS).[4,5] In the present work, an actinic pump pulse is introduced to record time-resolved Raman spectra. The intensity of the NCs mode is decreased while the hexane mode is increased as a function of time, which indicates that after photoexcitation, the NCs release energy through phonon modes to the solvents.

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Lead Free Zero-Dimensional Highly Luminescent Double Perovskite

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Lead-halide-perovskites (LHP), though having excellent optical properties,[1] limits their versatile applications due to (a) low ambient stability and (b) environmental sustainability because of toxic Pb.[2,3] As a model toxic-metal-free-perovskite (TMFP) system, $Cs_2InBr_5.H_2O$ has been adopted. Zero-dimensional structure of this TMFP system was confirmed from single crystal X -ray diffraction (SCXRD) analysis. However, this TMFP system has low PLQY (6%). But, enhancement of PLQY (λ_{em}^{max}: 695 nm) to 80% was observed upon 1% Sb^{3+} doping (Figure 1b). Moreover, this Sb^{3+} doped TMFP system is highly stable at ambient condition and SCXRD analysis supports the zero-dimensional structure for Sb-doped TMFP system (Figure 1a). Presence of multiple excited state in this Sb-doped TMFP system could be evidenced through temperature dependent PL measurements (80K – 300K) (Figure 1c). High value of exciton binding energy (78 – 115 meV) in these TMFP systems indicates less diffusive nature of the excitons. Moderate extent of electron-phonon coupling has been confirmed from Huang-Rhys-factor (~41) calculation.[4] The excited state lifetime of Sb-doped TMFP systems were observed to be long (~2.3 µs). It was calculated that Sb^{3+} doping enhances the radiative rate constant ~11 times and decrease the non-radiative rate constants ~3 times (Figure 1d).

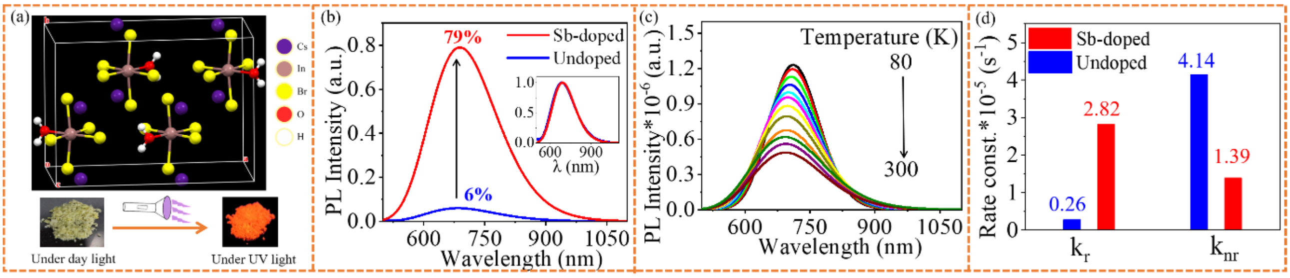

Figure 1: (a) Crystal structure, photo under day light and UV light of Sb^{3+}-doped TMFP, (b) PL emission of undoped and Sb^{3+}- doped TMFP (inset showing unchanged PL peak position upon Sb^{3+} doping),(c) Temperature dependent PL emission for Sb^{3+}-doped TMFP, (d) k_r and k_{nr} for undoped and Sb^{3+}- doped TMFP.

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Lead Free Double Perovskite: White Light Emission With 98% PLQY

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Lead-halide-perovskites have excellent optical properties,[1] however, their applications are limited due to (a) low ambient stability and (b) environmental sustainability concern because of the presence of toxic Pb.[2,] As a model lead-free-halide-perovskite (LFHP) system, $Cs_2NaInCl_6$ has been adopted due to robust 3D perovskite structure & high ambient air stability[3]. Undoped $Cs_2NaInCl_6$ shows very weak PL emission (photoluminescence quantum yield (PLQY)= 0.84%). However, doping of low amount (1.6%, obtained from ICPMS) of Sb^{3+} yields dual emission (peaks at 450 and 580 nm) (Figure 1a) and enhances the PLQY to 98%. Identical PXRD pattern observed for undoped as well as 1.6% Sb-doped LFHP system showed similar crystalline nature for both these systems. ICPMS, EDAX and XPS analyses confirm the presence of Sb^{3+} in the crystal. λ_{ex} dependent PL emission spectra of Sb-doped LFHP system showed predominantly yellow emission for λ_{ex}: 280-300 nm and predominantly blue emission for λ_{ex}: 320-350 nm. However, with λ_{ex}: 310 nm, a white light PL emission with PLQY: 98% was observed with CIE coordinate of 0.33,0.32 (Figure 1b), signifying near pure white emission. With increasing monitoring wavelength from 450 nm to 580 nm, the excited state lifetime was increased from 1.5 μs to 4.8 μs.

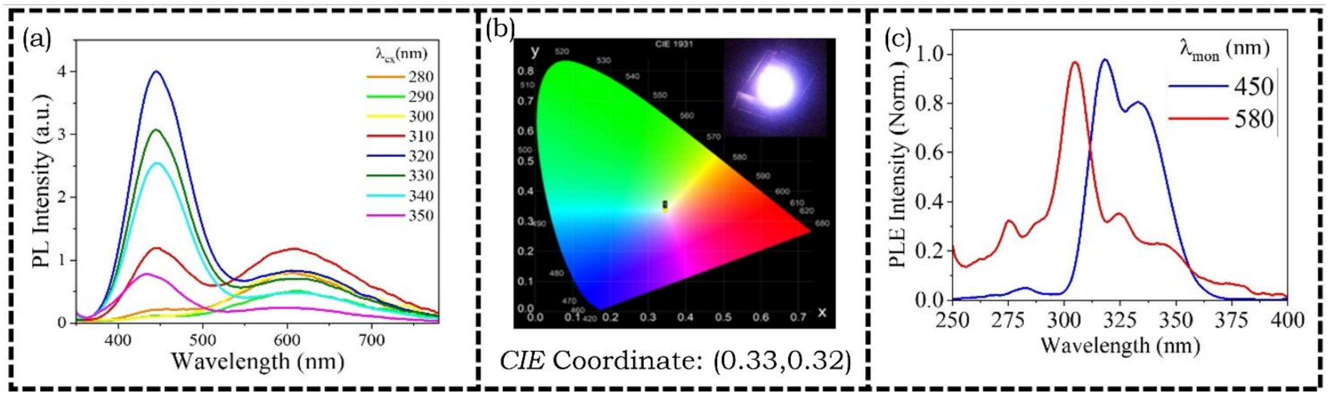

Figure 2: (a) PL emission of Sb^{3+}- doped $Cs_2NaInCl_6$ at different excitation wavelength (b) CIE coordinate (λ_{ex} = 310 nm) (c) Excitation spectra of Sb^{3+}-doped $Cs_2NaInCl_6$.

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Thickness Driven Plexciton Dynamics in Au@$CsPbBr_3$ Nanoplatelets

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Exploitation of plasmonic metal/perovskite hybrid materials for solar energy conversion is largely unexplored despite perovskite nanocrystals (NCs) already establishing remarkable position in the field of energy research, their applications ranging from photovoltaics to optoelectronics.[1] A previous paper from our group briefly discussed plasmonic perovskite hybrid nanomaterials and their exciton- plasmon interaction. The paper discusses how localized surface plasmon resonance (LSPR) of Au along with simultaneous exciton resonance from the semiconductor $CsPbBr_3$ NCs enhances the light absorption to many folds, covering the entire visible region of the absorption spectra, making it vital for solar energy conversion.[2] In this work, we synthesize $CsPbBr_3$ nanoplatelets with tunable thickness leading to variable exciton binding energies, thereby showing exciting interaction with the plasmon. We report observation of plexcitons in Au hybrid $CsPbBr_3$ nanoplatelets using optical spectroscopic measurements. Owing to the fact that exciton binding energy (E_b) increases with reduced thickness in nanoplatelets, emerging from both quantum and dielectric confinement present in low dimensional materials, enhancing the Fröhlich interaction.[3] This leads to enhanced exciton-phonon scattering, dominating the exciton decay kinetics of the system. Au incorporation in thin $CsPbBr_3$ NPls completely suppresses exciton–phonon scattering, enabling strong plexciton formation via coupling between Au plasmons and confined excitons. This unique observation can be highly promising and emphasize their relevance in non-linear optoelectronics.[4]

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Observation of Giant Rabi Splitting in Ag@CsPbCl3 Nanohybrids

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Surface plasmon resonance (SPR) in metallic nanoparticles such as Ag and Au provides an effective approach to manipulating light–matter interactions and enhancing energy transfer in hybrid nanostructures. When coupled with semiconductors, the broad plasmonic absorption band of metal nanoparticles can overlap with the sharp excitonic absorption peak of perovskites, giving rise to exciton–plasmon interactions of varying strength.[1] Unlike conventional semiconductors limited by deep traps, lead-halide perovskites exhibit shallow traps that suppress non-radiative recombination and enable efficient charge transport.[2] By constructing Ag@$CsPbCl_3$ hybrid nanostructures, we observed a modified absorption response, where the plasmon resonance red-shifts to lower energy and the excitonic transition blue-shifts to higher energy. This opposite-direction movement results in Rabi splitting, with the formation of upper and lower polaritonic branches.[3-4] Such spectral modifications unlock important properties, where exciton–plasmon coupling governs carrier relaxation, energy transfer pathways, and exciton dynamics. Importantly, the coupling strength is not fixed but can be tuned by external parameters. Two effective control routes are demonstrated here: (i) the concentration of $CsPbCl_3$ nanocrystals, where higher concentrations increase exciton density and enhance coupling, while lower concentrations weaken it; and (ii) halide substitution within the perovskite lattice, where exchange from Cl^- to Br^- modifies the excitonic resonance relative to the plasmon band, reducing spectral overlap and thus decreasing the interaction. Together, these tuning strategies establish perovskite–metal nanostructures as versatile platforms for regulating light–matter coupling, offering new opportunities for solar energy conversion, excitonic energy transport, and advanced optoelectronic applications.

Keywords: Surface plasmon resonance, Rabi splitting, Ag@$CsPbCl_3$, Coupling tune, Energy transfer

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Superstructures of Copper Nanoclusters as NIR TADF Emitters: Solvent-Dependent Optical and Morphological Modulation

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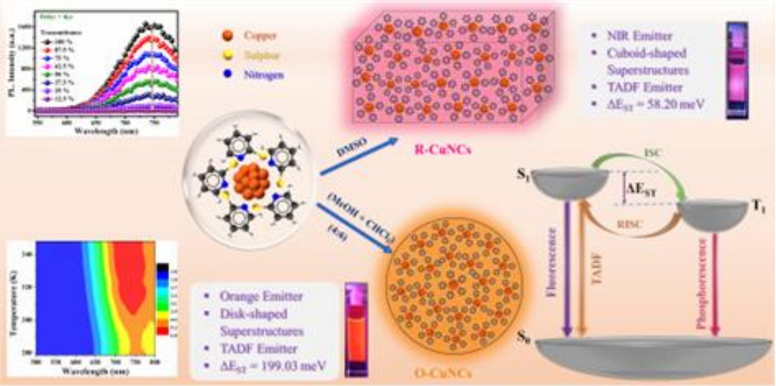
Thermally Activated Delayed Fluorescence (TADF) in nanomaterials accompanied by an NIR emission is an emerging research theme because of its extensive array of applications in optoelectronics. TADF is a rare and fragile phenomenon that balances an ethereal equilibrium between singlet-triplet state, spin-orbit couplings, balanced contribution of charge transfer and locally excited states. Stabilising the TADF emitters to harvest energy from the singlet and triplet state requires embedding them in a solid-state matrix, which is quite challenging for Metal nanoclusters (MNCs). The formation of the superstructures of MNCs can surpass this hurdle.[1-2] Herein, we report 2-mercaptopyridine-templated copper nanoclusters (CuNCs) which display near infrared (NIR) emission, both in the solid and colloidal states, as a result of the TADF (singlet-triplet energy gap, $\Delta E_{S1\text{-}T1}$ = 58.2 meV), which can be modulated to orange emission by preparing in a mixed solvent system of chloroform and methanol. Moreover, the solvent-dependent morphological tuning of the nanocluster superstructures, rendering a drastic change in the photo-physical signatures, is the consequence of different $\Delta E_{S1\text{-}T1}$ values for the CuNCs in different solvent environments.[3]



Scheme. Tuning of the superstructures of CuNCs in different solvent systems.

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Polaron-Mediated Energy Transfer and Exciton Dynamics in PANI–ZnO Nanocomposite Thin Films for PLED Emissive Layer

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This work investigates how controlled variation of polaron concentration within polyaniline (PANI) governs the excitonic behaviour and interfacial energy-transfer dynamics of PANI–ZnO nanocomposite thin films. Electropolymerized films on ITO-coated glass substrate exhibit distinct Grazing Incidence X-ray Diffraction peaks at small angles ($2\theta \approx 5$–$10°$), revealing semicrystalline ordering. Scanning electron microscopy analysis confirms uniform nanoscale dispersion of ZnO within the PANI matrix, establishing the spatial coupling required for Förster resonance energy transfer (FRET), with ZnO nanoparticles functioning as exciton donors and PANI hosting polaronic acceptor states[1]. Raman and photoelectron spectroscopy confirm the evolution of PANI into increasingly polaron-rich emeraldine structures as polaron concentration increases, which alters the polymer's electronic density of states and spectral overlap with ZnO emission. Optical absorption studies show that increasing polaron concentration widens the apparent optical band gap and reduces the Urbach energy, reflecting a reduction in electronic disorder and suppression of band-gap tail states that typically facilitate nonradiative decay. Photoluminescence spectra exhibit a polaron-dependent balance between ZnO emission quenching—signifying efficient donor-to-acceptor energy transfer—and emission enhancement when polaron density modifies recombination pathways[2]. These results establish polaron concentration as a fundamental control parameter for tailoring exciton dynamics, interfacial coupling, and radiative efficiency in PANI–ZnO for emissive layers in polymer light-emitting diodes (PLEDs).

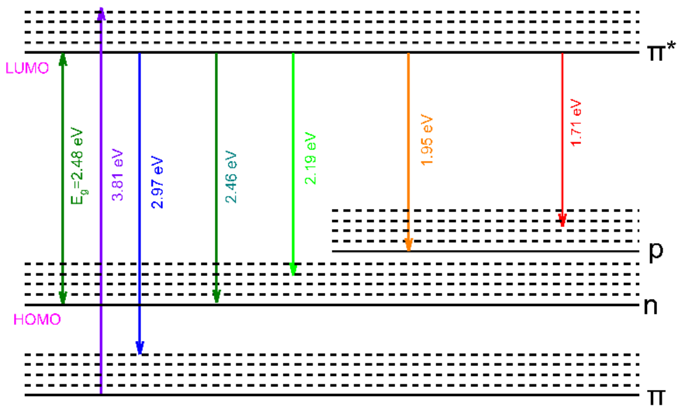

Figure: Schematic energy level diagram for PANI-ZnO nanocomposite thin film.

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Influence of Acid Dopants on Polaron Formation and Photophysical Response Correlated Nano-Structural Evolution in PPy–PMMA Blend Films for PLED Application

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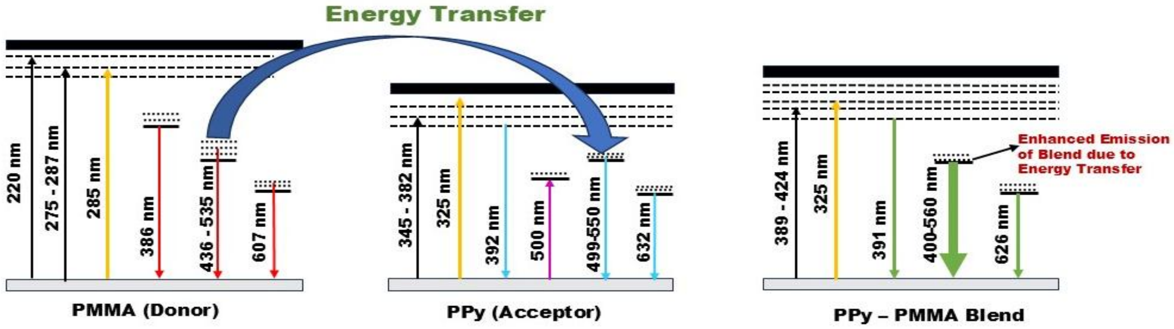
Polypyrrole-Poly(methyl methacrylate) (PPy-PMMA) polymer blend thin films doped with various inorganic acids have been deposited on indium tin oxide (ITO) coated glass substrates by electro-polymerization method. The significant changes in absorption and photoluminescence (PL) emission profiles of PPy-PMMA blends synthesized by varying acids signify the correlation between the generated polarons[1] and excitons in the blends. The maximum emission intensity was observed in sulfuric acid doped blend around 500 nm. The calculated band gap values were 1.91 eV, 1.78 eV and 1.72 eV for the blends doped with phosphoric acid, sulfuric acid and hydrochloric acid respectively. The microstructural images from scanning electron microscopy revealed boulder like structures of PMMA that were embedded in the nano globular form of PPy. The effective blending of PMMA with PPy in the thin films and the presence of vibrational modes of several characteristic functional groups (C=O, C-C-O, O-CH_3 etc.) were confirmed through the Raman spectroscopy. The luminescence enhancement in the blend may be ascribed to (a) efficient energy transfer from donor PMMA to acceptor PPy that enhances the overall emission[2] intensity of PPy, (b) formation of polaronic and bipolaronic states in between the HOMO-LUMO gap, which increases the formation of the singlet exciton leading to an intense emission spectrum. Hence the present work demonstrates that the incorporation of various acidic environment affects the luminescence of the polymer blends where the sulfuric acid doped PPy-PMMA blend can be used as a potential material for emissive layer in application of PLED.



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Quantifying Dexter Energy Transfer from Extra Faceted Perovskite Nanocrystal to Organic Dyes

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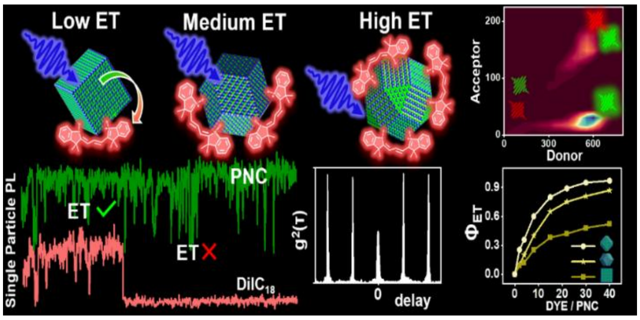
The surface structure of nanocrystals plays a critical role in how they interact with molecules at their interface.[1]We explore energy transfer (ET) from $CsPbBr_3$ perovskite nanocrystals (PNCs) with different shapes ranging from simple cubes to highly faceted nanocrystals to organic dye molecules. Ensemble photoluminescence measurements show that ET efficiency steadily increases with the number of facets, even though the overall surface area remains nearly constant. This suggests that extra facets provide more favourable binding sites for dyes in ensemble studies.[1,2]

To go beyond ensemble averages, we performed single-particle spectroscopy and these measurements reveal that the efficiency of ET per dye molecule is nearly the same for all PNC shapes. The higher overall efficiency observed in facet-rich PNCs for ensemble studies therefore arises not from efficient transfer dynamics, but from the fact that more dye molecules can attach to their surfaces.[3] Fluorescence correlation spectroscopy (FCS) further supports stronger dye association in solution. Together, these results show that Dexter-type ET dominates, enabled by dyes that directly anchor onto the PNC surface.[3]

Our study demonstrates that single-particle experiments are essential to disentangle molecular binding from intrinsic transfer rates, and that facet engineering offers a straightforward route to improve interfacial coupling in light-harvesting, sensing, and catalytic systems.



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Wave Function Engineering for Generating Long-Lived Hot Excitons

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The highly energetic excitons generated in a semiconductor nanocrystal, under supra-band edge excitations, are expected to be persistent due to the weak exciton-phonon coupling, generating a phonon bottleneck.[1] Contrary to the expected results, ultrafast cooling is observed in these quantum-confined systems, often attributed to the efficient Auger-type energy transfer between the coupled electron and hole in the hot excitons. Previous studies have established the influence of confinement and hole decoupling on intra-band cooling in quantum dots, further concretizing the notion of Auger-type energy transfer.[2,3] Herein, we modulate the electron wave function in hot excitons through suitable band-gap engineering in CdSe-based core–shell heterostructures, enabling a detailed understanding of hot-carrier cooling kinetics using transient absorption spectroscopy. We further extend these investigations to hot-electron extraction using an external acceptor, with the aim of harvesting the excess energy of hot electrons without energy loss, thereby advancing their potential for photovoltaic applications.

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Enhancing Plasmonic Photocatalysis Through Ligand Engineering

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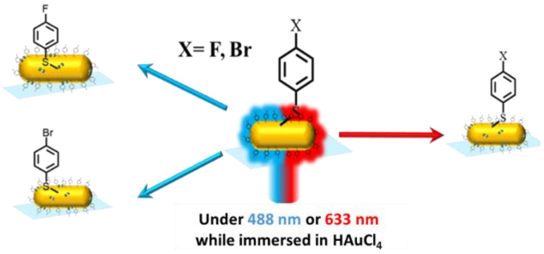
Plasmonic metal nanoparticles hold great potential for catalysis and photovoltaic applications due to their ability to concentrate electromagnetic energy and generate energetic hot carriers upon light excitation. However, their overall efficiency is often limited by the ultrafast recombination of these carriers within the metal. Coupling nanoparticles with species possessing vacant orbitals can facilitate charge separation by capturing one of the hot carriers, allowing the other to participate in subsequent chemical reactions.[1] In this study, gold nanorods (AuNRs) functionalized with 4-fluorothiophenol (4-FTP) and 4-bromothiophenol (4-BrTP) were investigated to assess their charge-separation efficiency. The reaction kinetics were monitored by tracking Au^{3+} reduction on individual nanorods under both interband and intraband excitation using dark-field scattering spectroscopy. Remarkably, under interband excitation, the photoinduced reduction of Au^{3+} on 4-FTP–functionalized nanorods was about 32 times faster than that observed on 4-BrTP–functionalized counterparts. In contrast, both ligand systems exhibited negligible activity under intraband excitation. Density functional theory (DFT) calculations revealed that the enhanced reactivity for 4-FTP arises from favorable hot-hole transfer from the gold d-band to the 4-FTP highest occupied molecular orbital (HOMO), leading to efficient hot-electron retention on the Au surface for catalysis. This ligand-mediated strategy offers a simple and cost-effective alternative to complex fabrication approaches that rely on coupling gold with other metals or semiconductors. Furthermore, the broad diversity of organic ligands provides a versatile platform for tuning charge-carrier dynamics.[2] Overall, these results underscore the importance of ligand design in promoting charge separation and offer mechanistic insights for the rational development of efficient plasmonic photocatalysts.



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Ultrathin Stoichiometric $CuInSe_2$ Nanoplatelets for Bioimaging Applications

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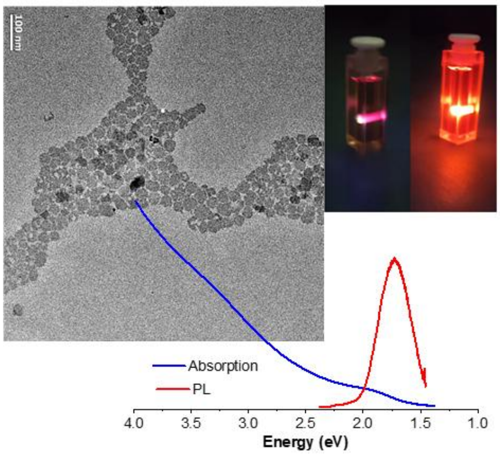
Copper indium selenide ($CuInSe_2$), a low-toxicity I-III-VI semiconductor, offers a promising alternative to conventional cadmium- and lead-based quantum dots for biological imaging. Two-dimensional (2D) nanocrystals (NCs) based on II-VI semiconductors are well known for their superior optical behavior and widespread applicability, suggesting that analogous I-III-VI-based NCs could provide similarly valuable functionalities. This motivates the development of innovative synthetic strategies targeting 2D I-III-VI nanostructures. Here, we present a phosphine-free colloidal synthesis route for 2D $CuInSe_2$ nanoplatelets (NPLs) with tunable optical properties. The NPLs were synthesized using a heat-up colloidal method, involving the formation of a Cu-In-Se lamellar template followed by crystallization of the constituent elements during the growth phase at 180°C. By carefully controlling precursor ratios, reaction temperature, and alloying conditions, we obtained phase-pure, stoichiometric $CuInSe_2$ NPLs while preserving their ultrathin morphology.

To enhance emission efficiency and biocompatibility, we engineered a $CuInSe_2$/ZnS core/shell heterostructure that provides effective surface passivation and significantly increased photoluminescence intensity. The resulting NPLs exhibit bright, narrow-band emission and excellent colloidal stability in aqueous media, making them suitable for biological environments. Their reduced toxicity, strong fluorescence, and robust dispersion enabled successful in vitro bioimaging, where clear intracellular fluorescence was observed without affecting cell viability. Overall, this study emphasises the significance of composition control and surface passivation in tailoring the optical properties of 2D $CuInSe_2$ NPLs, thereby establishing them as promising next-generation fluorescent probes for bioimaging and related optoelectronic applications.



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How to Slow down Phase Transformation of $CsPbBr_3$ Nanocrystals in Aqueous Medium? Playing with Metal Ion Hydration Energy

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Halide perovskites are game changers in the field of solar energy harvesting and optoelectronics. Yet, the soft and highly ionic nature of halide perovskites render them water and moisture unstable via non-perovskite phase transformation. Introducing nanoconfined aqueous metal halides having different hydration energy using a reverse micellar route, we are able to critically control the perovskite nanocrystals (NCs) to non-perovskite phase transformation. The nanoconfined aqueous monovalent NaCl salt preferentially first phase transforms $CsPbBr_3$ to $CsPb_2Br_5$, and then the Br → Cl exchange process starts to form $CsPb_2Cl_5$ NCs within just ~2 h of interaction. In contrast, the trivalent $AlCl_3$ salt first transforms $CsPbBr_3$ to $CsPbCl_3$, and is followed by complete phase transformation to $CsPb_2Cl_5$ NCs in a ~7-day duration. Here, the smaller hydration energy of Na^+ ion leads to easy release of water molecules, causing fast $CsPb_2Br_5$ transformation via CsBr stripping in water. Conversely, the very large hydration energy of the Al^{3+} ion holds the water molecules more firmly, resulting in an extremely slow phase transformation. Overall, we use a very fundamental concept of metal ion hydration energy for efficient prevention of the detrimental non-perovskite phase transformation in the aqueous environment, thus advancing towards sustainable optoelectronic applications of perovskite NCs.

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A Unified Chemical Approach That Simultaneously Addresses The Bottlenecks of Water Stability, Direct Dopability, and Thermal Robustness in Fragile Perovskite Nanocrystals

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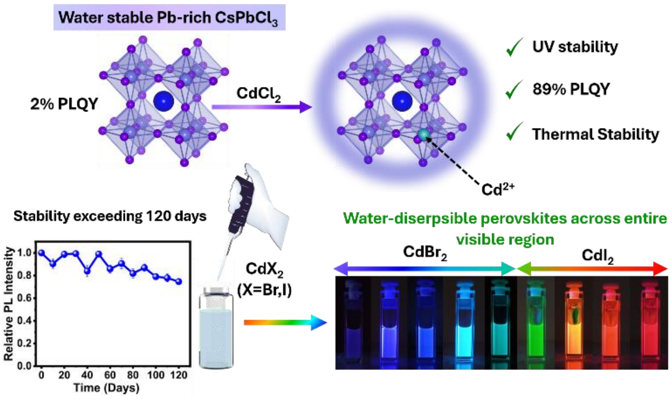

Despite the remarkable rise of halide perovskites in optoelectronics, their vulnerability to water and the lack of efficient blue emitters have remained long-standing barriers to practical implementation. Among all compositions, $CsPbCl_3$ is particularly challenging, although its wide bandgap is ideal for blue emission, it suffers from pronounced structural fragility, halide-vacancy traps, and incompatibility with polar media. Here, we report a unified design principle that transforms this inherent weakness into a functional advantage. By introducing a Pb-enriched surface and employing a dual-site ligand, (11-mercaptoundecyl)-N,N,N-trimethylammonium bromide (MUTAB), we achieve water-stable $CsPbCl_3$ nanocrystals that remain colloidally stable for over 120 days. The MUTAB ligand simultaneously anchors through Pb–S coordination and shields the lattice through electrostatic hydration away from the surface. This water dispersibility facilitates direct aqueous doping with CdX_2 (X = Cl, Br, I), allowing for facile lattice doping and halide exchange without post-synthetic processing, yielding near-unity photoluminescence quantum yield (~89%), reduced lattice disorder and blue emission that withstands UV and thermal stress. The discovery not only advances the chemistry of perovskite–water interfaces but also paves the way toward scalable, moisture-resistant blue LEDs and full-color optoelectronic devices.

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Tuning The Optoelectronic Properties of $MoSe_2$ Nanosheets Through Heterostructure Formation with Ag_2Se Nanocrystals

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Heterostructure engineering is a powerful strategy for overcoming the intrinsic trade-off between spectral range and carrier transport in photodetectors.[1] Here, we demonstrate a broadband, solution-processable photodetector based on a two-dimensional $MoSe_2$–Ag_2Se heterostructure, which integrates the strong visible absorption and high photogain of semiconducting 2H-$MoSe_2$ with the narrow-bandgap, high-mobility characteristics of Ag_2Se.[2] Structural analysis by X-ray diffraction and transmission electron microscopy confirms intimate heterointerfacing without compromising crystallinity. The resulting type-II band alignment enables ultrafast electron transfer from $MoSe_2$ to Ag_2Se and efficient hole confinement in $MoSe_2$, thereby promoting long-lived carrier populations. Devices exhibit a broad spectral response from 400 nm to 900 nm, a peak responsivity of 1.2 A W^{-1} at -3 V bias, a high detectivity of 8.5×10^{10} Jones, and rise/decay times of 150/268 ms. The synergistic combination of broadband absorption, low dark current, and efficient charge extraction highlights the $MoSe_2$–Ag_2Se heterostructure as a promising candidate for next-generation, low-cost, and scalable photodetection technologies.

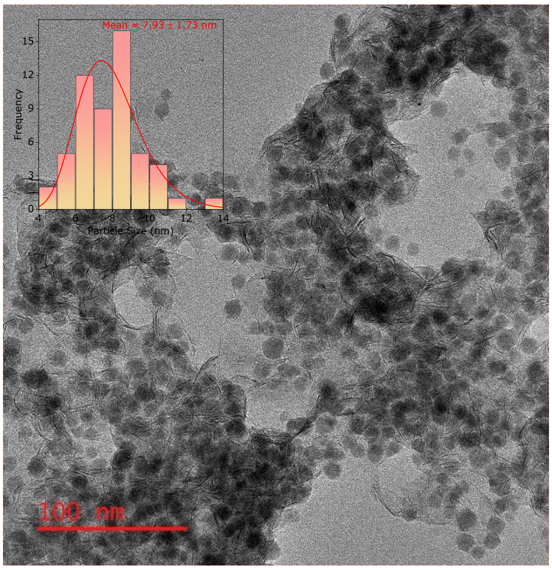

Figure 1. TEM image showing Ag_2Se nanoparticles uniformly distributed on $MoSe_2$ sheet.

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Intrinsic vs. Extrinsic STE Emission Enhancement in *ns*^{2} Ion Doped Metal (Cd, In) Halide Hybrids

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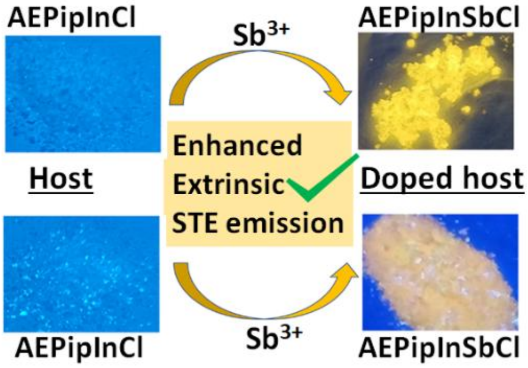
Broadband emission in zero-dimensional metal halide hybrids (Sb^{3+}, In^{3+}, Cd^{2+}, Bi^{3+}) arises from exciton self-trapping within metal-halide units (intrinsic STEs). Introducing extrinsic ns^2 ion-based dopants, such as Sb^{3+}, into Cd halide hosts (Rb_4CdCl_6), has been claimed to enhance intrinsic STE emission by softening the lattice.[1] However, similar photophysical properties of Cd hosts and Sb^{3+} dopants obscure the emission's nature. This study presents doped Cd and In-based metal halide hybrids, clarifying that enhanced emission results from dopant extrinsic STE, supported by photoluminescence quantum yield dependence on doping efficiency. Distinct excitation-dependent emission in hosts, compared to excitation-independent emission in doped systems, differentiates intrinsic and extrinsic STE, shedding light on emission mechanisms.



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Synthesis of Lead-Free Halide Perovskite Nanocrystals for White Light Emission

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Lead free lanthanide-based perovskite nanocrystals are emerging as promising material for highly stable and excellent optoelectronic behaviour.[1] In this work, we report the synthesis of Cesium Terbium Chloride (Cs_3TbCl_6) nanocrystals using standard hot injection synthesis route. The synthesized nanocrystals were phase-pure, uniform and monodisperse nanoparticles which was confirmed from X-ray diffraction and Transmission Electron Microscopy. We have obtained core-shell nanocrystals which shows difference in their morphology and size with different quenching temperatures such as 120 °C, 160 °C and 200 °C during the synthesis process. Photoluminescence studies show broad white emission under UV excitation wavelength and difference in PL intensity was observed for samples quenched at different temperatures. Furthermore, the nanocrystals show excellent stability in ambient conditions and maintained strong luminescence for several days. These results highlight the potential of Cs_3TbCl_6 nanocrystals as a robust and lead-free alternative for next-generation displays[1], X-ray imaging[1], light-emitting diodes[1], and other device applications.

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Facet-Engineered Rubidium Lead Halide Nanocrystals for Pyro-Phototronic Broadband Photodetection

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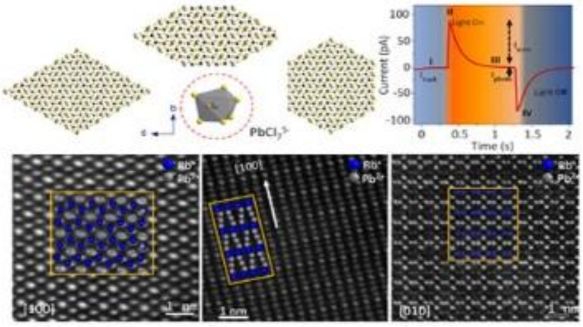
Cesium lead halide has been extensively studied as efficient materials for optoelectronic device applications. Beyond Cs(I), the exploration of other inorganic A-site monovalent cations remains limited, though Rb(I) stands out as a potential alternative whose role in colloidal nanocrystals is largely unexplored. Here, Rb (I) is employed as an effective A-site cation in forming monoclinic-phase $RbPb_2Cl_5$, where Pb (II) heptahedrally coordinated. A template mediated cation exchange strategy is employed where 0D Rb_4CdCl_6 used as host nanocrystals. Upon introduction of Pb (II), fast Cd to Pb ion exchange triggers and 2D $RbPb_2Cl_5$ in rhombic prism, hexagonal prism or hexagonal platelet shaped nanocrystals are formed depending on the reaction conditions. Further to explore the optoelectronic properties, photo response measurements are carried out which exhibit significant pyro-photocurrent response from these nanocrystals even under ultra-low-intensity light illumination (7 nW/cm^2) across ultraviolet (UV) to near-infrared (NIR) spectral range. Despite its centrosymmetric structure, $RbPb_2Cl_5$ generates pyro-photocurrent due to surface halide deficiencies, supported by DFT showing surface polarization of $|\mathbf{\Delta}P| = 0.173$ C/m^2. These findings highlight the pivotal role of Rb (I) in stabilizing these nanostructures and open a new avenue for their application in advanced optoelectronic devices.



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Tuning The Reaction Chemistry for The Sulfo-Bromination of Bismuth, Leading to Dual-Tapered Bi-Sulfobromide Platelet Nanocrystals and Their Heterostructures

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The chemistry of sulfo-bromination of metals leading to dual-tapered 2D-shaped nanostructures is reported. This has been confined to the metal ion Bi(III), whose reduction followed by reionization in the presence of sulfide and bromide precursors leads to the desired bismuth sulfobromide nanocrystals. Initially $Bi_{19}S_{27}Br_3$ seed rods are taken, where Bi(0) nanocrystals are connected via a redox chemistry, conjugating with secondary metal ions. Then these 1D-shaped $Bi_{19}S_{27}Br_3$–Bi(0) heterostructures are transformed to dual-tapered 2D-shaped $Bi_{19}S_{27}Br_3$–Bi(0) nanostructures following a solution–liquid–solid (SLS) growth mechanism. The sulfo-bromination process is initially nucleated on the metal(0) sites but grown on the surface of the substrate seed rods. The size of Bi(0) equilibrates the tapering, whereby the length of the rods is gradually reduced and the width of the rods is slowly widened, leading to the dual-tapered 1D to 2D shape transferred Bi-chalcohalide nanostructures. Extensive electron microscopic analysis and stepwise synthesis have been carried out to investigate the growth mechanism and to understand the tapering during the shape evolution processes. In addition, these materials of seed rods, intermediate and final nanostructures obtained are further explored as photocatalysts for HER and their activities are compared. The reaction chemistry discussed here enables the controlled incorporation of two anions with Bi(0) ionization, where one end of the nanostructure initiates nucleation, while the other end promotes growth. Overall, the reaction chemistry here provides a pathway for the solution-processed 2D SLS growth process, leading to shape-controlled metal chalcohalide nanostructures.

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Atomically Precise Nanoclusters as Pressure Sensors

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Atomically precise metal nanoclusters (APMNCs) are emerging as model systems for solid-state photophysics and stimuli-responsive luminescent materials, yet their behavior under extreme pressure remains poorly understood.[1-4] Here, we establish carborane-thiolate-protected Cu_4 clusters, Cu_4@oCBT, Cu_4@mCBT, and Cu_4@ICBT, as intrinsic pressure probes. Combining in situ photoluminescence, Raman spectroscopy, powder X-ray diffraction, and first-principles DFT up to ~10 GPa, we disentangle ligand-controlled structural and electronic responses in these molecular solids. All three crystals display intense room-temperature phosphorescence that increases upon compression, followed by quenching beyond a ligand-dependent threshold. Cu_4@oCBT and Cu_4@mCBT exhibit the expected red-shift of emission, whereas iodinated Cu_4@ICBT shows an unusual initial blue-shift before reverting to red-shift, indicative of pressure-tuned competition between emissive states. Three characteristic regimes emerge: (i) a sub-GPa ligand-reorientation window, (ii) a 3–5 GPa metal core deformation, and (iii) amorphization above ~7–8 GPa, each mirrored in Raman mode parameters and DFT band-gap evolution. These results, placed in the context of recent high-pressure studies on Au/Ag clusters and piezochromic Cu_4 systems, demonstrate that the carborane shell acts as a mechanical transducer, converting hydrostatic stress into programmable optical outputs. The work provides a design blueprint for cluster-based, high-gain, pressure-responsive phosphors and calibrants.

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Dots to Dye: Tunable Carbon Quantum Dots for Efficient and Safe Imaging Across Biological Systems

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Carbon Quantum Dots (CQDs) is emerging as a rapidly growing area of research owing to their exceptional photoluminescent properties, adjustable surface functionalities, and outstanding biocompatibility. In this study, CQDs were produced using microwave heating method with urea and citric acid in three distinct concentrations. The structural, morphological, optical, electrochemical and surface properties of the synthesized CQDs were extensively characterized using selected characterization techniques. The fluorescence emission of CQDs was found to vary with urea concentration, revealing a correlation between nitrogen doping and amorphous carbon structure formation. The biocompatibility and toxicity of CQDs were evaluated using *Drosophila melanogaster* as an *in vivo* model, where concentration-dependent effects on development and survival were observed. Additionally, CQDs demonstrated efficient cellular uptake and bright fluorescence in Drosophila salivary glands, confirming their potential for bioimaging. In plant systems, CQDs were successfully utilized for section imaging, providing enhanced contrast and visualization of cellular structures under UV excitation without the need for conventional dyes. Overall, the study highlights the dual applicability of CQDs in animal and plant systems, emphasizing their potential in bioimaging, nanotoxicology, and sustainable nanobiotechnology.

Keywords: Carbon Quantum Dots (CQDs), Drosophila, Plant, Bioimaging

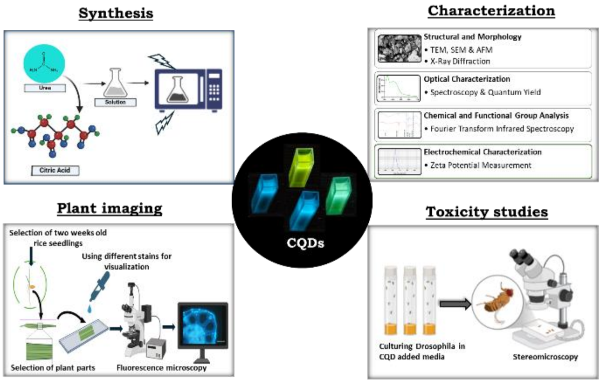

Figure 1. Graphical abstract

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Conjugated Polymers for Stable and Delocalized Polarons

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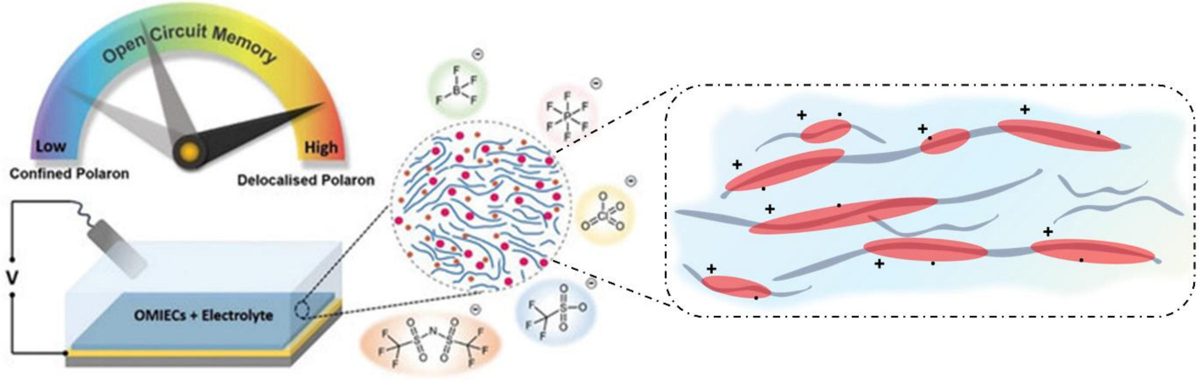
Organic semiconductors have emerged as promising materials for flexible optoelectronic devices and bioelectronic sensors. However, their device performance hinges on the nature of polarons generated through chemical or electrochemical doping. Doping enhances conductivity, but the resulting polarons are localized due to structural and energetic disorder in conjugated polymers. Despite decades of research, fundamental questions about the spin characteristics, energy levels, and spatial delocalization of polarons remain unresolved.

In our research, we explore the electronic structure and dynamics of polarons in doped conjugated polymers, highlighting recent spectroscopic and theoretical insights into their nature. Building on these findings, molecular design strategies are proposed to stabilize polarons and promote long-range delocalization through tailored backbone planarity, side-chain engineering, and dopant–polymer interactions. These approaches offer a framework for improving charge transport, optical modulation, and stability in functional organic electronic materials.



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Rational Design of NIR-Emissive RTP-TADF AIEgens for Enhance Type II ROS Generation in Photodynamic Cancer Therapy

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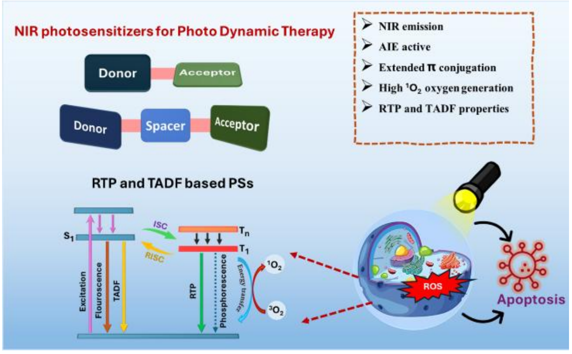
Image-guided photodynamic therapy (PDT) is emerging as a powerful cancer treatment strategy that offers minimal systemic toxicity while enabling real-time visualization of therapeutic response. Although thermally activated delayed fluorescence (TADF) and room-temperature phosphorescence (RTP) materials have shown growing potential in PDT, their distinct contributions to reactive oxygen species (ROS) generation and phototherapeutic outcomes remain insufficiently understood. In this work, a series of NIR-emissive, AIE-active, metal-free photosensitizers were rationally designed by tuning the substitution pattern on the molecular core, resulting in controlled variations in molecular conformation and excited-state properties. These structural modifications tailored key photophysical parameters including ΔEST, ISC/RISC dynamics, spin-orbit coupling, radiative decay rates, and triplet-state character enabling a switch between TADF and RTP behavior. The materials exhibit strong NIR emission and generate efficient ROS under light irradiation, supporting their suitability for image-guided PDT. Systematic comparison of the TADF and RTP active systems reveals clear differences in ROS generation pathways, triplet-exciton utilization, and light-induced cytotoxicity in cancer cells. The combination of AIE characteristics, tunable triplet-state properties, and NIR emission within a single molecular platform presents a promising strategy for advancing high-performance, metal-free photosensitizers for precise and effective PDT. This study highlights the potential of molecular engineering in developing next-generation organic systems for image-guided cancer therapy.



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Naphthalimide Derivatives as Potent Type 1 ROS Generators for Potential Photodynamic Therapy Applications

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Cancer affects millions of people globally, making it a critical area of focus for researchers, clinicians, and public health officials. Photodynamic therapy is a clinically approved anticancer modality that employs a light activated agent (photosensitizer) to generate cytotoxic reactive oxygen species (ROS).[1] There is therefore a growing interest for developing innovative photosensitizing agents with enhanced phototherapeutic performances. In this study, we synthesized and characterized a series of 6 novel naphthalimide derivatives to evaluate their potential as Type 1 ROS generators under photodynamic conditions. The synthesized compounds were subjected to in vitro photophysical and photochemical analyses to assess their ROS generation capabilities. Our results demonstrated that these naphthalimide derivatives efficiently produce Type 1 ROS, which was confirmed by using different chemical trapping assays. Additionally, these Photosensitizers are designed in a way that they are cell organelle targeting which will be beneficial for targeted cancer therapy and can be used for bio-imaging. Given their efficient ROS generation, the synthesized compounds show great promise as photosensitizers for PDT.

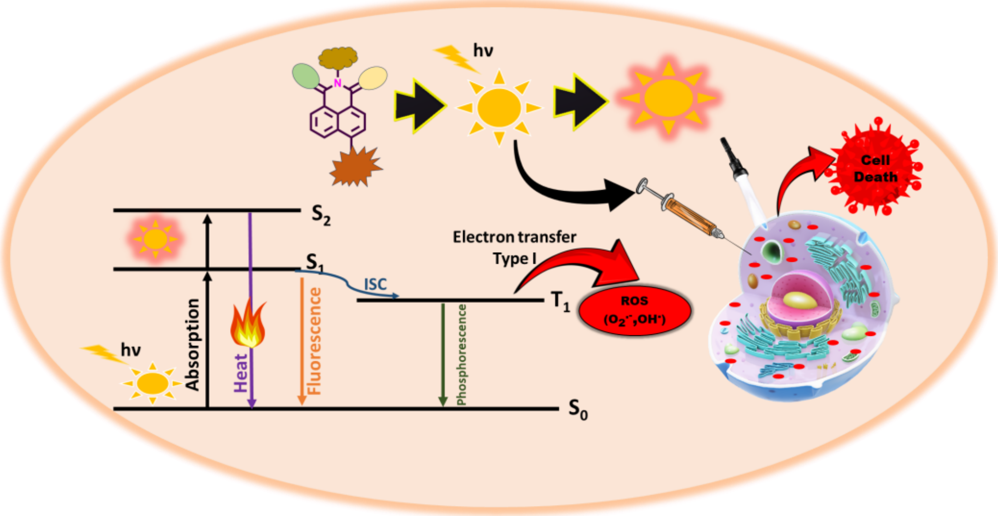

Fig 1. Schematic illustration of Photo Dynamic Therapy through Type I mechanism.

Future research will focus on exploring their therapeutic efficacy in *in vivo* models. The findings suggest that with further development, these compounds could become valuable tools in the advancement of photodynamic therapy for cancer treatment.

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Mapping The Structural Features of FUS: from Isolated Molecules over Oligomers to Phase-Separated Condensates

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The Intrinsically Disordered Protein (IDP), FUS (Fused in Sarcoma), forms biomolecular condensates that are directly linked to neurodegenerative disorders, including Amyotrophic Lateral Sclerosis (ALS) and Frontotemporal Dementia (FTD). Despite their biological significance, the conformational properties of individual FUS molecules remain poorly understood due to their structural heterogeneity, environmental sensitivity, and in-chain complex dynamics. Using biophysical techniques such as Multiparameter Fluorescence Detection (MFD), we map the pathway from flexible FUS monomers to nanoclusters and fibrillar assemblies. Our findings indicate that pFCS detects a salt-dependent expansion of isolated FUS molecules and a 200–400 µs timescale structural relaxation. Analyses of various FUS fragments and variants have helped elucidate the compactness of the native-length FUS protein by deciphering the intra- and intermolecular interactions that underlie its packing. smFRET and eTCSPC data reveal a quasi-continuum of relaxation times of FUS, underscoring that IDPs are not random coils but dynamic ensembles. Below the saturation concentration (C_{sat}), FUS forms reversible oligomers and clusters that compact, align, and grow autocatalytically-processes suppressed by RNA. Above C_{sat}, FUS assembles into condensates featuring nanometer-scale meshwork that progressively matures into heterogeneous droplets and fibrils. These findings map a quantitative framework for IDP assembly and prioritize early metastable states for intervention.[1-3]

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Mapping Ultrafast Relaxation Dynamics of Large Stokes Shift Red Fluorescent Protein

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Red fluorescent proteins with large Stokes shifts (LSS-RFP) are highly advantageous for fluorescence imaging owing to their substantial spectral separation and reduced self-absorption[1,2]. Among these LSS-RFPs, LSSmKate1, LSSmKate2 and mBeRFP are widely used in multicolor bioimaging due to their high brightness, photostability, efficient maturation, low cytotoxicity, and pH stability[3,4]. However, a complete understanding of excited-state processes and their photophysics is still lacking, necessitating a comprehensive investigation. In this work, we use a combination of spectroscopic and computational methods to investigate a possible role of excited-state proton transfer (ESPT) in the LSS of these LSS-RFPs under varying temperature and isotopic conditions. This study demonstrates that ESPT occurs faster in LSSmKate1 than in LSSmKate2 and we also discuss temperature-dependent local and distant emissions, along with dual and triple fluorescence in mBeRFP[5], the first known case of triple fluorescence in a fluorescent protein. In summary, we proposed a model to uncover the underlined intricate excited state photophysical behaviour of these LSS-RFPs.

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Oxidative Stress Amplifying Norbornene-Based Polymeric Nanocarrier for Bioimaging-Based Multidrug-Resistant Cancer Chemotherapy

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Multidrug resistance (MDR) remains a major obstacle in achieving effective cancer chemotherapy, often leading to treatment failure and tumor relapse. In this work, we developed a multifunctional norbornene-based amphiphilic nanocarrier using ring-opening metathesis polymerization (ROMP) of functionalized norbornene monomers incorporating reactive oxygen species (ROS)-generating moieties to amplify oxidative stress and enable site-specific, on-demand drug release in MDR tumor cells. The nanocarrier self-assembles into core–shell structures, with a hydrophobic norbornene-derived core for drug loading and a hydrophilic corona for stability and circulation. Doxorubicin-dichloroacetate (DOX-DCA) was efficiently encapsulated within the hydrophobic core through a self-assembly process, yielding nanoparticles with uniform morphology and high drug loading efficiency. Once accumulated at the tumor site via avidin-biotin interactions and enhanced permeability and retention (EPR) effect, the system promotes intracellular ROS amplification, triggering rapid destabilization of the nanostructure. In vitro studies show that the nanocarrier bypasses efflux pumps, increases intracellular drug retention and enhances cytotoxicity compared to free drug toward resistant cancer cells. Additionally, DCA disrupts mitochondrial metabolism, further increasing ROS levels and sensitizing cancer cells to DOX induces synergistic apoptosis. This oxidative stress-amplifying nanocarrier encapsulated with chemotherapeutics offers a promising route for precision chemotherapy against MDR cancers.

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Polynorbornene Conjugated Hyperbranched Networks: A Soft Luminescent Polymer Platform for Potential Bio-fouling Applications

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Bio-fouling is an undesirable phenomenon that occurs when microorganisms, plants, and animals congregate and colonize on wetted material surfaces and surfaces exposed to humid environments.[1] It poses major threat to the marine, health and food industries, as well as water treatment systems. Conventional anti-fouling agents used widely in the last decade were mostly made of toxic metals and organic/hydrophobic biocides posing serious threat to the ecosystem. Due to environmental concerns, non-toxic anti-fouling materials based on amphiphilic/hydrophilic polymer hydrogels have been chosen.[2] The hydrophilicity provides the ability to resist nonspecific protein adsorption and cell adhesion by forming a hydration layer, preventing the attachment of biological materials. Hyperbranched polyglycerols (HPGs) have evolved as a suitable candidate for designing hydrophilic polymer materials, owing to their dense -OH branching, biocompatibility, versatility and tunability.[3] However, multifunctionality and long-term stability still remains a challenge. Polynorbornenes have been known to be highly rigid polymers with excellent mechanical properties. Thus, we have designed an HPG-grafted polynorbornene system to utilize their synergy in providing a robust material that combines mechanical strength, chemical resistance, surface functionality, and durability. The architecture also provides an unusual CTE-based emission which further improves the material's cause as a soft material coating for biomedical applications.

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Installation of Cationic Phosphorous on Dimethyldihydropyrene Photoswitches: An Alternative Approach Towards Efficient Far-Red Photoswitching in Water

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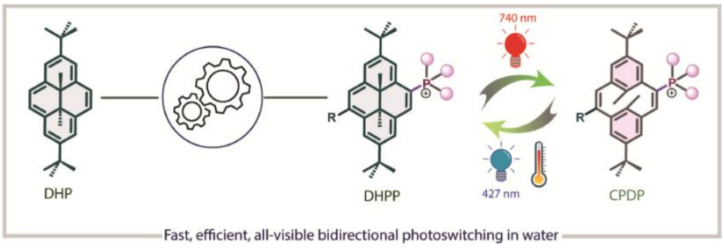
In the rapidly evolving field of photochromic material applications in biological systems,[1] there is an urgent need for the development of multi-stimuli-responsive, biocompatible systems. Conventional organic photochromic systems are often lipophilic and use UV-light in at least one of the bidirectional switching. Negative (inverse) photoswitches that undergo switching from a thermally stable coloured state to a metastable colourless state offer additional advantages over their positive counterparts in terms of enhanced optical transparency and increased penetration depth during photo-irradiation. Herein, we have synthesised a library of negative photochromic dimethyldihydropyrene phosphonium salts, which can be activated by red and far-red (up to 740 nm) photons in a quantitative manner in the "biological window".[2] The intriguing feature of this particular modification is the remarkable improvement in the response time, with a substantially improved ring-opening quantum yield than that of the conventional DHP system with fully aqueous operation. Furthermore, the reversal can be achieved upon exposure to visible light and also under thermal conditions in a quantitative manner, thereby enabling fully bidirectional visible light-mediated switching. Importantly, the tunable thermal half-lives of the metastable isomers make this particular class of photoswitches even more versatile, a potentially promising candidate for prospective applications in biological systems.



Fast, efficient, all-visible bidirectional photoswitching in water

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Spacer-Mediated Interplay of Triplet Excitons in Delayed Fluorescent Emitters

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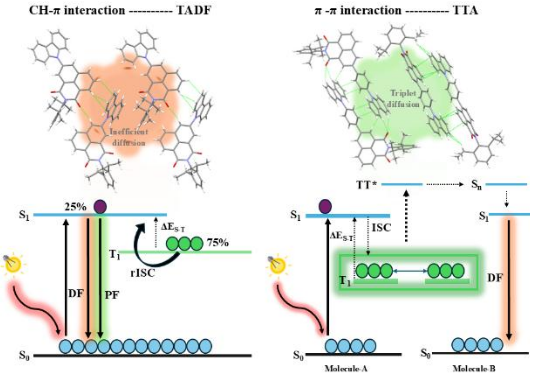
Designing organic emitters that maintain efficient delayed fluorescence in the solid state remains a significant challenge for practical device applications.[1] Although both TADF and TTA offer routes to recycle triplet excitons, their activation is highly sensitive to molecular packing, conformational freedom, and host–guest interactions in solid films.[2] Polymer matrices often introduce energetic disorder and restrict molecular motion, leading to the simultaneous presence of multiple emissive species such as locally excited states, charge-transfer states, and excimer/aggregate states.[3] Herein, we have designed two molecules for TADF and two for TTA by using naphthalimide (**NI**) derivative as an acceptor and N-phenyl carbazole (**PhCBZ**) or carbazole (**CBZ**) as a donor at 5,6-position of naphthalimide moiety. Thin films of the CBZ and PhCBZ-substituted naphthalimides doped in the poly(methyl methacrylate) (**PMMA**) matrix exhibit TADF emission and TTA-induced delayed emission respectively. The subtle structural modification alters intermolecular p-p and CH-p interactions, directing PhCBZ-substituted molecules toward a TTA pathway while CBZ-substituted analogues predominantly exhibit TADF.[4]



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Non-Conventional Clusteroluminescence from Unconjugated Poly(2,3-dihydrofuran)

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In recent times, non-conventional luminescent polymers have emerged as attractive alternatives to traditional fluorescent materials.[1] While conventional systems achieve fluorescence through π-conjugated frameworks or established chromophores, these polymers generate emission through entirely non-conjugated structures. In this work, we present a new class of non-conjugated, emissive polymers derived from 2,3-dihydrofuran (DHF). Poly(2,3-dihydrofuran) (PDHF) samples with different molecular weights were synthesized through cationic polymerization and were found to emit brightly in both solution and solid states (Figure 1). The excitation-dependent emission of PDHF indicates the existence of several distinct emissive states, in contrast to conventional fluorophores that maintain fixed electronic states.[2] While dilute solutions show weak luminescence, the intensity increases with concentration, indicating the absence of aggregation-caused quenching (ACQ).[3] Furthermore, adding non-solvents such as hexane or water to PDHF solutions in THF significantly enhances fluorescence, confirming aggregation-induced emission (AIE).[3] Beyond their luminescent properties, PDHF films exhibit excellent transparency in the visible region. They appear invisible under ambient light yet emit strong fluorescence under UV, enabling applications in invisible inks, anti-counterfeiting, data encryption, and smart labeling.

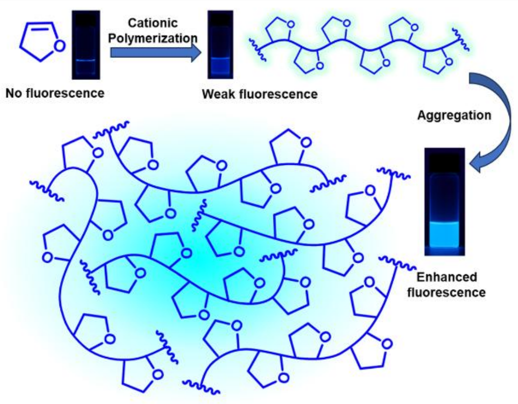

Figure 1. Nonconventional luminescence behavior of PDHF.

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Clustering-Induced Emission of Maleimide-Based Homopolymers

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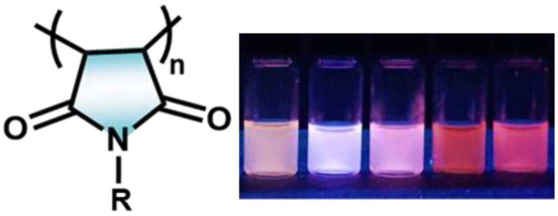
Stimuli-responsive polymers capable of translating environmental changes into measurable optical or phase transitions are of growing interest for sensing, smart materials, and soft-matter applications.[1] Among these, systems that exhibit non-conventional emission (NCE) without classical chromophores offer unique opportunities for designing simple yet multifunctional polymer platforms. In this work, a series of maleimide-based homopolymers were synthesized via free-radical polymerization to investigate their unusual photophysical and environmental responsiveness. The densely packed maleimide units enable distinct NCE behavior arising from through-space electronic interactions. Beyond their emission properties, these homopolymers show sensitivity to external stimuli, including pH-induced fluorescence modulation and thermally triggered transitions. Notably, specific derivatives exhibit pronounced upper critical solution temperature (UCST)–type thermoresponsiveness that drives reversible self-coacervation through cosolvency-mediated aggregation. Together, these findings demonstrate that structurally simple maleimide homopolymers can serve as versatile, stimuli-adaptive materials with promising potential in sensing, separation, and responsive soft-matter systems.



Clusturization triggered emission and coacervate formation

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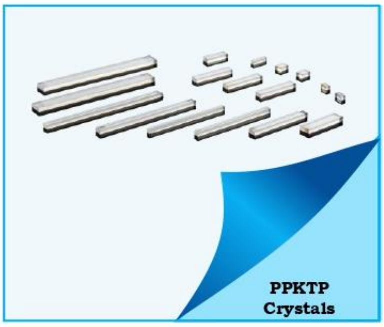
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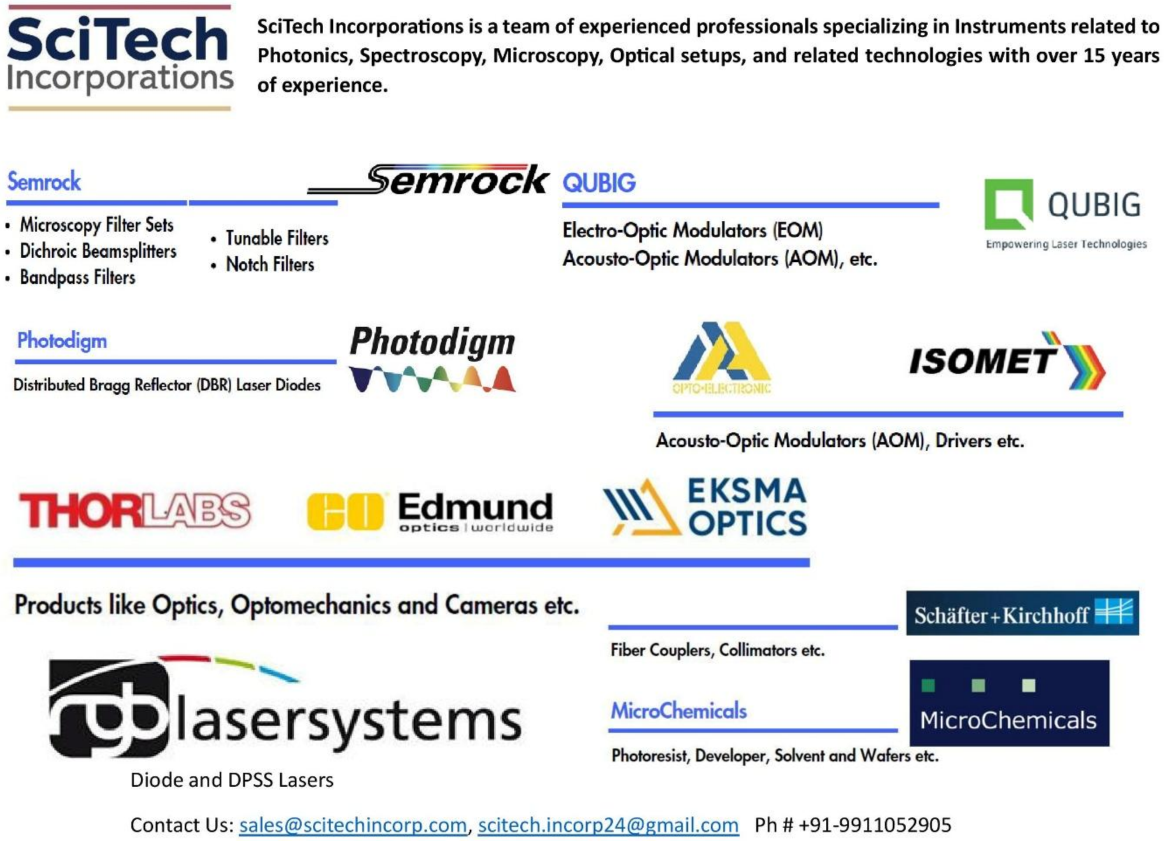
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