Nanomaterials and **Mo**lecules: From **S**pectroscopy to **Bio**imaging

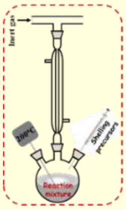
(**NaMoSBio**)

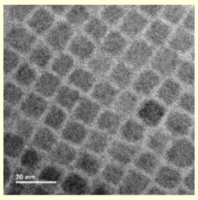
An International Conference

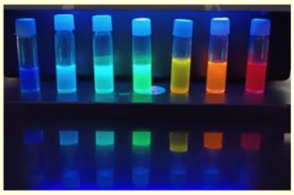
@

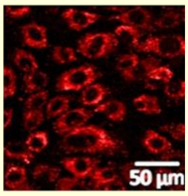
R N Tagore Auditorium, IISER Kolkata

12-14 January, 2024









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INDIAN INSTITUTE OF SCIENCE EDUCATION & RESEARCH (IISER) - KOLKATA
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IISER Kolkata, India, 10-01-2024

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**)" in the IISER Kolkata campus during January 12-14, 2024.

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,

Soumitro Banerjee
Director, IISER Kolkata

निदेशक/Director
भारतीय विज्ञान शिक्षा एवं अनुसंधान संस्थान कोलकाता
Indian Institute of Science Education and Research Kolkata
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भारत सरकार के मानव संसाधन विकास मंत्रालय द्वारा स्थापित एक स्वायत्तशासी संस्थान
INDIAN INSTITUTE OF SCIENCE EDUCATION & RESEARCH (IISER) - KOLKATA
Established by the Ministry of Human Resource Development (MHRD), (An Autonomus Institution, Government of India).

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IISER Kolkata, India, 10-01-2024

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**)" during January 12-14, 2024.

This International Conference is intended to provide a suitable platform for cutting-edge research problems related to optical nanomaterials and molecules, synthesis, spectroscopy-dynamics 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 from listening to the stalwarts in these research fields.

I wish this International Conference a great success.

Sincerely,

Debasish Haldar

Debasish Halder
DCS Chairperson, IISER Kolkata

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INDIAN INSTITUTE OF SCIENCE EDUCATION & RESEARCH (IISER) - KOLKATA
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Dr. Prasun K. Mandal, Ph.D.
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IISER Kolkata, India, 10-01-2024

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**)” at IISER Kolkata during January 12-14, 2024.

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 17 lecture sessions, comprising of 3 Plenary Lectures, 1 Special Evening Lecture, 6 Keynote Lectures, 23 Invited Lectures and more interestingly, 6 young researchers will deliver the cutting-edge research of their early career in a special session called “Young-Investigators’ Flash Presentation”. Around 55 senior graduate students will present posters in the poster session on January 13, 2024.

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 are introducing 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 spite of their busy 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
Convenor, **NaMoSBio** International Conference
On behalf of the Organizing Committee of **NaMoSBio** 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), 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 symbiosis.

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:

IISER Kolkata is a leading research institute in India, dedicated to advancing research in multidisciplinary sciences. The Department of Chemical Sciences (DCS) at IISER Kolkata, which is one of the first departments to be established in IISER Kolkata, has been at the forefront of this effort. From the beginning, the Department has incarnated the Institute's mission of excellence in both research and teaching. Its recent works demonstrate its commitment to cutting-edge research in various fields of chemistry. 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.

Tentative schedule of the programme:

Day 1: 12th January 2024, Friday		
07:30-09:00	Registration at R. N. Tagore Auditorium	
09:00-09:30	Inauguration & Welcome address	
Session 1 Chair: Sushanta Dattagupta, Founding director, IISER Kolkata, India		
09:30-10:15	Plenary lecture 1	*Speaker:* D. D. Sarma, IISc Bangalore, India *Title*: Dynamics of Photoluminescence in Mn-Doped Pb-Halide Perovskite Nanocrystals
Break		
Session 2 Chair: Priyadarsi De, IISER Kolkata, India		
10:25-11:00	Keynote lecture 1	*Speaker:* Don C. Lamb, LMU München, Germany *Title*: Extracting Kinetics using Single Molecule FRET
11:00-11:20	Invited lecture 1	*Speaker:* Arindam Chowdhury, IIT Bombay, India *Title*: Probing Local Surface Polarity of (Bio)molecular Aggregates using Sensitized Emission Imaging
11:20-11:40	Tea Break	
Session 3 Chair: Ayan Datta, IACS Kolkata, India		
11:40-12:15	Keynote lecture 2	*Speaker:* Narayan Pradhan, IACS Kolkata, India *Title*: Color Tunable Quantum Dots: Seeing from Reaction Flask to Watching those under Electron Microscope
12:15-12:35	Invited lecture 2	*Speaker:* Pankaj Mandal, IISER Pune, India *Title*: 1D Lead Halide Perovskites for Nonlinear Optics and Photonics
12:35-12:55	Invited lecture 3	*Speaker:* Sayan Bagchi, CSIR-NCL Pune, India *Title*: Surface-Ligand Interactions in Quantum Dots: 2D IR Insights
12:55-14:15	Lunch Break	
Session 4 Chair: Sanjib Bagchi, IISER Kolkata, India		
14:15-14:35	Invited lecture 4	*Speaker:* Subhajit Bandyopadhyay, IISER Kolkata, India *Title*: Light-Switches in Biomimetic Catalysis
14:35-14:55	Invited lecture 5	*Speaker:* Sanchita Sengupta, IISER Mohali, India *Title*: Diindolocarbazole-Based Twisted Organic TADF Triads and Donor-Acceptor Compounds for Efficient Energy- and Electron-Transfer Photocatalysis
14:55-15:15	Invited lecture 6	*Speaker:* Debapratim Das, IIT Guwahati, India *Title*: From Molecule to Material: The Case of an Ultrashort Peptide
15:15-15:35	Invited lecture 7	*Speaker:* Apurba Lal Koner, IISER Bhopal, India *Title*: Styryl-Based Far-Red Emissive Fluorogenic Probes for Biological Applications
15:35-15:55	Invited lecture 8	*Speaker:* Sarit S. Agasti, JNCASR Bangalore, India *Title*: Single Molecule Imaging through Engineered Molecular Interaction
15:55-16:20	High Tea	
Session 5 Chair: Arabinda Chaudhuri, IISER Kolkata, India		

16:20-16:40	Invited lecture 9	*Speaker:* Anindya Datta, IIT Bombay, India *Title*: Strategies and Challenges in Engineering the Excited State Processes of Fluorogenic Molecules
16:40-17:00	Invited lecture 10	*Speaker:* Soumen Ghosh, IISc Bangalore, India *Title*: Time-Domain Broadband Circular Dichroism Spectroscopy: A Novel Probe of Chiral Structure and Spin Dynamics
Break		
Session 6 (Young-Investigators' Flash Presentation) Chair: Pradipta Purkayastha, IISER Kolkata, India		
17:10-17:20	Flash Talk 1	*Speaker:* Satyajit Patra, BITS-Pilani, Pilani, India *Title*: Breaching the Diffraction Limit in Single Molecule Fluorescence Detection using Zero-Mode Waveguide (ZMW) Nanostructures
17:20-17:30	Flash Talk 2	*Speaker:* Navendu Mandal, Imperial College London, UK *Title*: Ultrafast Intraband Spectroscopy of Perovskite Systems: Extending the Defect Tolerance to Hot Carrier Cooling Dynamics
17:30-17:40	Flash Talk 3	*Speaker:* Kingshuk Mukhuti, Radboud University, Netherlands *Title*: Optically-Tracked Thermal-Breach-Memory in $\mathrm{MaPbI_3}$
Break		
Session 7 Chair: D. D. Sarma, IISc Bangalore, India		
17:45-18:30	Special Evening Lecture	*Speaker:* Sushanta Dattagupta, Founding director, IISER Kolkata, India *Title*: Nonlinear Optical Conductivity of Graphene and Related Phenomena
Break		
Session 8 Chair: Sanchita Sengupta, IISER Mohali, India		
19:00-19:05	Sponsor Talk 1	RSC
19:05-19:10	Sponsor Talk 2	Simco Global Technology & Systems Ltd. (Silver Sponsor)
19:10-19:15	Sponsor Talk 3	Advanced Photonics (Silver Sponsor)
19:15-19:20	Sponsor Talk 4	Specialise Instruments (Silver Sponsor)
19:20-19:25	Sponsor Talk 5	Laser Spectra Services (Bronze Sponsor)
19:30-22:00	Dinner	

Day 2: 13th January 2024, Saturday		
Session 9 Chair: Don C. Lamb, LMU München, Germany		
09:00-09:45	Plenary lecture 2	*Speaker*: K. George Thomas, IISER TVM, India *Title*: Semiconductor Quantum Dots: From Trap-States to Single Photon Purity
Break		
Session 10 Chair: Timothy W. Schmidt, UNSW, Australia		
09:55-10:30	Keynote lecture 3	*Speaker*: Ashok K. Ganguli, IIT Delhi and IISER Berhampur, India *Title*: Design of Nanomaterials for Energy Conversion, Storage and Medical Applications

10:30-11:05	Keynote lecture 4	*Speaker*: Peter Reiss, CEA, Grenoble, France *Title*: III-V Semiconductor Quantum Dots: Synthesis and Applications
11:05-11:30	Tea Break	
Session 11 Chair: Nitin Chattopadhyay, Jadavpur University, India		
11:30-11:50	Invited lecture 11	*Speaker*: Mahesh Hariharan, IISER TVM, India *Title*: Symmetry Breaking Charge Separation in Chromophoric Dimers
11:50-12:10	Invited lecture 12	*Speaker*: Jyotishman Dasgupta, TIFR Mumbai, India *Title*: Tracking Correlated Triplet-Triplet Pairs in Singlet Exciton Fission
12:10-12:30	Invited lecture 13	*Speaker*: Ratheesh K. Vijayaraghavan, IISER Kolkata, India *Title*: Engineered Solid-State Aggregates in Brickwork Stacks of n-type Organic Semiconductors: A Way to Achieve High Electron Mobility
12:30-13:00	Group Photo Session	
13:00-14:00	Lunch Break	
Session 12 Chair: Ranjit Biswas, SNBNCBS Kolkata, India		
14:00-14:35	Keynote lecture 5	*Speaker*: Achanta Venu Gopal, CSIR-NPL Delhi, India *Title*: Label-Free Single Molecule Sensing with Metamaterials
14:35-14:55	Invited lecture 14	*Speaker*: Nirmalya Ghosh, IISER Kolkata, India *Title*: Emerging Polarized Light Methodologies for Probing Nano Scale Structural Anisotropy
14:55-15:15	Invited lecture 15	*Speaker*: Satyaprasad P Senanayak, NISER Bhubaneswar, India *Title*: Electronic and Ionic Transport in Mixed Metal Perovskites
15:15-15:35	Invited lecture 16	*Speaker*: Pabitra K. Nayak, TIFR Hyderabad, India *Title*: Doping of Soft Semiconductors towards Stable and Efficient Optoelectronics
Break		
Session 13 Poster Judges: Jyotishman Dasgupta, Deepa Khushalani, Moloy Sarkar, Sanchita Sengupta, Satyajit Patra		
15:45-18:00	Poster presentation (with High Tea)	
Session 14 (Young-Investigators’ Flash Presentation) Chair: Asoke P. Chattopadhyay, University of Kalyani, India		
18:00-18:10	Flash Talk 4	*Speaker:* Anup Ghosh, SNBNCBS Kolkata, India *Title*: The Mechanistic Insights into Drug Carrier Development, Cell Penetration Mechanisms, and Target Binding Studies
18:10-18:20	Flash Talk 5	*Speaker:* Tushar Debnath, IIT Guwahati, India *Title*: Halide Driven Energy and/or Charge Transfer Dynamics in Perovskite Nanocomposite
18:20-18:30	Flash Talk 6	*Speaker:* Ganesh Agam, Cambridge, UK *Title*: How Robust is Studying the Structural Dynamics of Biomolecules by Single Molecule FRET Spectroscopy?
Break		
Session 15 Chair: Soumen Ghosh, IISc Bangalore, India		

18:35-18:50	Sponsor Talk 6	ATOS (Platinum Sponsor)
18:50-19:00	Sponsor Talk 7	Laser Science (Gold Sponsor)
19:30-22:00	Dinner	

Day 3: 14th January 2024, Sunday		
Session 16 Chair: K. George Thomas, IISER TVM, India		
09:00-09:45	Plenary lecture 3	*Speaker*: Anunay Samanta, University of Hyderabad, India *Title*: Charge Carrier Relaxation Dynamics in Perovskite Nanocrystals
Break		
Session 17 Chair: Chilla Malla Reddy, IISER Kolkata and IIT Hyderabad, India		
09:55-10:30	Keynote lecture 6	*Speaker*: Timothy W. Schmidt, UNSW, Australia *Title*: Pushing the Limits of Photochemical Upconversion
10:30-10:50	Invited lecture 17	*Speaker*: Anshu Pandey, IISc Bangalore, India *Title*: Electronic Structure and Optical Properties of I-III-VI$_2$ Semiconductor Quantum Dots
10:50-11:10	Invited lecture 18	*Speaker*: Sukhendu Nath, BARC Mumbai, India *Title*: Excited State Dynamics and their Role in Biosensing
11:10-11:30	Invited lecture 19	*Speaker*: Pramod P. Pillai, IISER Pune, India *Title*: Light-Matter Interactions at Nanoscale Leading to Chemical Changes
11:30-11:50	Tea Break	
Session 18 Chair: Sayam Sengupta, IISER Kolkata, India		
11:50-12:10	Invited lecture 20	*Speaker*: Jino George, IISER Mohali, India *Title*: Long-Range Energy Transfer in Strongly Coupled Systems
12:10-12:30	Invited lecture 21	*Speaker:* Deepa Kushalani, TIFR Mumbai, India *Title*: Concurrent Energy Capture and Storage - Route to Formation of Solar Batteries
12:30-12:50	Invited lecture 22	*Speaker*: Abhishek Dey, IACS Kolkata, India *Title*: Reduction of Sulfur Dioxide to Sulfur Monoxide by Ferrous Porphyrin
12:50-13:10	Invited lecture 23	*Speaker*: Moloy Sarkar, NISER Bhubaneswar, India *Title*: Fluorescent Copper Nanoclusters: A Versatile Candidate for Understanding its Interactions with Biologically and Environmentally Important Analytes
13:10-13:20	**Poster prize distribution** **by Prof. Sushanta Dattagupta, Prof. Anunay Samanta, Prof. Peter Reiss and Prof. Don C. Lamb**	
13:20-13:30	Valedictory followed by vote of thanks	
13:30-14:15	Lunch Break	
14:30	Departure of Faculty members for **Banquet Dinner**	
15:30	Departure of Students for **Banquet Dinner**	

Contents

Plenary Lectures

Dynamics of Photoluminescence in Mn-Doped Pb-Halide Perovskite Nanocrystals

D. D. Sarma

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Nanocrystals of lead halide perovskites have been shown to have extraordinary photoluminescence properties, spanning the entire visible range achieved by the composition tuning via solid solutions at the halide site. Taking cues from Mn doping of traditional Group II-VI semiconductor quantum dots, Mn doping of the lead halide perovskites has been extensively explored by the community, establishing intense Mn-dopant induced emission that is significantly Stokes shifted from the excitonic emissions of the host. While all reports agree on the essential features of this emission, such as the peak position and the width of the Mn photoluminescence, there appears to be little agreement on the microscopic processes by which the host sensitizes Mn following its photoexcitation and the steps that control the deexcitation leading to the Mn emission. There are even reports of disagreement between different reports on the temperature dependence of the Mn emission and its origin. I shall discuss the present status of this field and establish, with the help of new experimental data as well as the already reported ones, what appears to be the microscopic processes controlling the excited dynamics in the Mn-doped lead halide perovskites.

Bio-sketch

D. D. Sarma

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D. D. Sarma obtained a 5-year Integrated MSc (1977) in Physics from Indian Institute of Technology (IIT) Kanpur and a Ph.D. (1982) from Indian Institute of Science (IISc). He worked at Kernforschungsanlage Jülich as Visiting Scientist during 1984-1986. He was a faculty member at Solid State and Structural Chemistry Unit of IISc during 1986-2021. Presently, he is an Honorary Professor and CSIR Bhatnagar Fellow at IISc. His research interest spans the science of strongly correlated electron systems, semiconductor nanocrystals, and energy materials.

Semiconductor Quantum Dots: From Trap-States to Single Photon Purity

K. George Thomas

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The semiconductor quantum dots (QDs) at the single-particle level exhibit mysterious episodes of photoluminescence (PL) intermittency, often called PL blinking, represented by ON-, GRAY-, and OFF-states which occur due to the trapping of charge carriers and Auger recombination. The first part of the presentation will discuss single-particle charge carrier dynamics in various QDs by employing various time-resolved PL measurements and strategies for controlling the undesirable OFF-states. The second part of the presentation will explain our recent approaches for estimating single exciton and biexciton quantum yield in QDs and nanoplatelets, along with synthetic strategies for controlling exciton purity. The presentation will also cover newer strategies for enhancing the PL of QDs through plasmon resonance coupling.

Bio-sketch

K. George Thomas

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K. George Thomas is a Professor and J C Bose National Fellow at the School of Chemistry of the Indian Institute of Science Education and Research Thiruvananthapuram, India. Research activities of KGT group focus on understanding the photochemistry and photophysics of molecular assemblies, plasmonic systems, semiconductor quantum dots, and chiral nanostructures using various steady-state and time-resolved techniques. George Thomas is a recipient of several awards and fellowships: the most significant ones are the J C Bose National Fellowship (2014-2024), and the Shanti Swarup Bhatnagar Prize in Chemical Sciences (2006). He is an elected fellow of both the Indian National Science Academy, New Delhi (2015) and the Indian Academy of Sciences, Bangalore (2007). He was the President of the Asian and Oceanian Photochemistry Association (2019-2021) and was a member of the Editorial Advisory Committee of the Journal of Physical Chemistry of the American Chemical Society (2012-2015).

Charge Carrier Relaxation Dynamics in Perovskite Nanocrystals

Anunay Samanta

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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.[1,2] 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 very 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.[3-9]

References:

1. Dey, A.; *et al.* State of the art and prospects for halide perovskite nanocrystals. *ACS Nano* **2021**, *15*, 10775-10981.
2. Green, M. A.; Ho-Baillie, A.; Snaith, H. J. The Emergence of Perovskite Solar Cells. *Nat. Photonics* **2014**, *8*, 506-514.
3. Mondal, N; De, A.; Das, S.; Paul, S.; Samanta, A. Ultrafast carrier dynamics of metal halide perovskite nanocrystals and perovskite-composites. *Nanoscale* **2019**, *11*, 9796-9818.
4. Mondal, N; De, A.; Samanta, A. Achieving near-unity photoluminescence efficiency for blue-violet-emitting perovskite nanocrystals. *ACS Energy Lett.* **2018**, *4*, 32-39.
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Bio-sketch

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Anunay Samanta received his Ph.D. degree in 1987 from Indian Association for the Cultivation of Science (Jadavpur University) with Prof. Mihir Chowdhury. After a postdoctoral stint at the Radiation Laboratory, University of Notre Dame for a couple of years he joined the chemistry faculty at University of Hyderabad in early 1990, where he is currently a Senior Professor (re-employed). His current research interest lies in ultrafast dynamics and single-molecule spectroscopy of the perovskite nanocrystals. For his research contributions, Prof. Samanta has received many recognitions and awards. He has been elected to the Fellowship of all three National Science Academies. He is also a J.C. Bose National Fellow since 2009. He is a recipient of Thomson Reuters India Citation Award, Raman-Mizushima Lecture Award, APA Award, Prof. Masuhara Lectureship Award, Visitor's Award, Prof. Sadhan Basu Memorial Lecture Award, and many more.

Special Evening Lecture

Nonlinear Optical Conductivity of Graphene and Related Phenomena

Sushanta Dattagupta

Founding Director, IISER Kolkata, Mohanpur, Nadia 741246, West Bengal, India.

Graphene -- a wonder laboratory -- is a system with remarkable properties and applications. The essential quantum richness of the two-dimensional material that has earned itself the epithet of a Dirac solid, has been described in the literature. It turns out that the basic building blocks of graphene -- from the electronic configuration of a single carbon (C) atom -- to the hybridization of the orbitals of two nearest neighbour C atoms, yielding a honeycomb lattice in the tight-binding limit -- can be used to teach distinct aspects of master's level quantum mechanics, both relativistic and non-relativistic. After giving a pedagogical overview of these basic attributes, I will turn attention to the study of nonlinear optical conductivity of graphene. The optical absorption beyond the linear Drude-Kubo regime is investigated in terms of the familiar spin-boson model of quantum dissipation, in which the 'spin' refers to the two-state system of valence and conduction band wave functions for a given k-value of the momentum. The necessary formalism is based on the 'Rotating Wave Approximation' of Quantum Optics and the 'Master Equation' approach to non-equilibrium statistical mechanics. The different roles of phonons and electrons in inducing quantum dissipation and thereby optical absorption will be analyzed.and the results for spin-lattice and spin-spin relaxation rates will be graphically illustrated.

In the end, if time permits, I will discuss similar results in two dimensional oxide materials, on planar Hall effect and magneto resistance.

Bio-sketch

Sushanta Dattagupta

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A. Born: 19 December 1947

B. Education: (i) Undergraduate and Postgraduate Studies at Calcutta University (1962 - 68); (ii) Doctoral Studies at Brookhaven National Laboratory, New York (1969 - 73); Post-doctoral work at Carnegie-Mellon University, Pittsburgh (1973-75) and University of Alberta, Edmonton (1975-76).

C. Career: (i) Lecturer in Physics, Presidency College (1968- 69); (ii) Scientific Officer, Indira Gandhi Centre, Kalpakkam (1976 - 81); (iii) Reader in Physics, University of Hyderabad (1981- 86); (iii) Professor, School of Physical Sciences, JNU (1986 - 99); (iv) Director, S. N. Bose Centre (1999 - 2005); (v) Director, IISER Kolkata (2006 - 2011); (vi) Vice Chancellor, Visva-Bharati (2011 - 2016); (vii) Senior Scientist (2017 - 2022) and Honorary Scientist (2022-) of the Indian National Science Academy.

D. Fellowship: (i) Fellow of Indian Academy of Sciences (1992), Indian National Science Academy (1994), National Academy of Science (1995); (ii) Member of The World Academy of Science (TWAS) (1999).

E. Awards: (i) Young Scientist (1977) and C. V. Raman (2010) medals of INSA; (ii) C. V. Raman Birth Centenary Award of the Indian Science Congress (2006); (iii) M. N. Saha Memorial Award of the National Academy of Science (2005); (iv) Alexander von Humboldt Award at Juelich (1984); (v) Visiting Fellowship at Cavendish Laboratory of Cambridge University (summers of 1992 and 1994), Ben Gurion University, Beer Sheva, Israel (2008-2009) and Senior Associateship at ICTP, Trieste (1990 - 95); (vi) 'Sera Bangali' prize of the ABP Group (2012) and (vii) J. C. Bose Fellowship of the Department of Science and Technology (2006 - 2015).

F. Books: (i) Relaxation Phenomena in Condensed Matter, Academic Press (1987); (ii) Dissipative Phenomena in Condensed Matter Physics (with S. Puri), Springer-Verlag (2004); (iii) A Paradigm called Magnetism, World Scientific (2008); (iv) Diffusion -- Formalism and Applications, Taylor and Francis (2013); (v) 'Je Path Diye' (in Bengali), Visva-Bharati publications (2014); (vi) A Random Walk in Santiniketan Ashram, Niyogi publishers (2015); (vii) Visva-Bharati 1921 - 2021: A Vision Betrayed, THEMA (2021).

G. Research Interest: (i) Relaxation and Spectroscopy, (ii) Dissipation and Diffusion, (iii) Magnetism, (iv) Quantum Dissipation, (v) Quantum Nano Materials, (vi) Science Education.

Keynote Lectures

Extracting Kinetics using Single Molecule FRET

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Förster Resonance Energy Transfer (FRET) experiments can be used to probe interactions, conformations and dynamics on the nanometer scale with single-molecule sensitivity. Hence, it is well suited for investigating biomolecules and biomolecular interactions. Recently, a multilaboratory study showed that single-molecule FRET (smFRET) experiments can be reproducibly measured and dynamics detected on the subnanometer scale.[1] By expanding the number of fluorophores used for smFRET measurements to three, it is possible to detect conformation changes induced upon binding, follow FRET between two acceptors or to measure three distances simultaneously. For solution-based smFRET experiments, we have developed a three-color photon distribution analysis approach.[2] In the case of immobilized molecules, we developed a Deep-Learning Assisted Single molecule Image analysis (Deep-LASI) approach. The Deep-LASI software performs an automated trace characterization and kinetic analysis of single-molecule intensity traces. With this approach, it is now possible to analyze intensity traces in minutes rather than days.[3]

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3. Wanninger, S. *et al.* Deep-LASI: deep-learning assisted, single-molecule imaging analysis of multi-color DNA origami structures. *Nat. Commun.* **2023**, *14*, 6564.

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Don C. Lamb is currently Professor for Biophysical Chemistry at the Ludwig-Maximilians-University Munich. He studied Mathematics and Physics at Illinois Wesleyan University and obtained a PhD in Physics from the University of Illinois at Urbana-Champaign under the supervision of Professor Hans Frauenfelder. Before moving to Munich, Professor Lamb worked as a research fellow jointly at Vanderbilt University, Massachusetts General Hospital and Harvard Medical School, was an Alexander von Humboldt Research Fellow at the Technical University of Munich, Germany, spent three years at the Laboratory for Fluorescence Dynamics in Urbana-Champaign, IL USA and was a visiting scientist at the University of Ulm, Germany.

The research of Professor Lamb focuses on the development and application of fluorescence methods. He is well known for his contributions to single molecule Förster Resonance Energy Transfer (smFRET) experiments and Fluorescence Fluctuation Spectroscopy, in particular with the development of Pulsed Interleaved Excitation. He has applied smFRET for investigating the conformation and dynamics of several protein systems including chaperone proteins. Other areas of expertise include fluctuation imaging, single particle tracking and studies of viral entry, assembly and release.

Color Tunable Quantum Dots: Seeing from Reaction Flask to Watching those under Electron Microscope

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Semiconducting nanocrystals are widely known for their color tunable bright emissions. Varying the composition or size, the bandgap of these nanocrystals varies and this tunes their emission colors. The color may be tuned with change in size or composition. 2023 Noble Prize of chemistry also associated with the Chemistry of formation of these nanocrystals. This talk will present the basics of quantum dots, controlling their color tunability and brightening factors, images under electron microscope and also their potential applications. The excitement of a chemist from preparing those in reaction flask to see those under electron microscope will be narrated. Ligands, facets and dimension tunable shape/size which control such nanocrystals brightness will also be discussed. The development of chemistry from 1990 to 2023 will be presented with progress of the basic understanding from their formation to stability. This will cover both chalcogenide and perovskite quantum dots.

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Narayan Pradhan is currently working as a Professor in Indian Association for the Cultivation of Science. He did PhD from IIT Kharagpur and post docs from Israel and USA before he joined at IACS in 2007. He works on chemistry and physics of inorganic semiconductor nanocrystals.

Design of Nanomaterials for Energy Conversion, Storage and Medical Applications

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Coupling of wide band gap semiconductors such as nanostructured ZnO, $NaNbO_3$ with narrow band gap semiconductors like nanostructured Ag_2S, In_2S_3, $CuInS_2$ (which act as sensitizers) form efficient heterostructures for solar energy conversion.[1] We have reported[2] Mn doped $BiVO_4$ to improve the charge-transport properties of the catalyst for enhancing efficiency of conversion. Synthesis of transition metal dichalcogenides and their heterostructures(especially with rGO), MoS_2/VS_4/rGO, MoS_2/rGO/Cu_2O and SnS_2/TaS_2/rGO have been designed for efficient photoelectrochemical and photodetector applications[3-6].

Among energy storage devices, batteries and supercapacitors have been of major interest. Sodium-ion batteries are the next-generation and cost-effective alternative to the presently rechargeable lithium-ion batteries owing to their vast abundance. We report[7] the improvement in the electrochemical performance via incorporating vanadium in $Na_2Ti_3O_7$. We have also explored electrochemical performance of $Na_2Ti_3O_7$ (NTO) with multiwalled carbon nanotubes (CNT) as an anode in Li-ion coin cells[8].

Yb^{3+}-Tm^{3+} doped $NaBiF_4$ based upconversion nanomaterials have been designed for bioimaging of cells[9]. Methylene blue loaded $K_{0.3}Bi_{0.7}F_{2.4}$: Yb, Er upconversion nanoparticles have been designed for near-Infrared activated photodynamic therapy[10]. We have also designed Ln^{3+} (Ln = Tb, Gd) ions doped $NaBiF_4$(NBF) and $K_{0.3}$Bi0.7$F_{2.4}$ (KBF) nanoparticles as nanoscintillators for high resolution X- ray imaging[11]. We also discuss design of surface - modified silica nanoparticles in drug delivery enhancing drug loading, controlled release, and therapeutic efficacy. These virus-mimicking, spiky silica nanoparticles with MOFs (Metal-Organic Frameworks) like ZIF-8/ZIF-90, imparting pH-responsive properties enables the selective release of payloads in appropriate environment[12,13].

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Professor Ganguli is currently the Director and Professor of Chemical Sciences at IISER Berhampur. He is on Lien from IIT Delhi where he is a Professor of Chemistry. He was Deputy Director, IIT Delhi and was also the founding Director of Institute of Nano Science and Technology (Mohali, India). He studied in University of Delhi (BSc and MSc) and obtained his PhD from SSCU, IISc Bangalore in 1990. He worked at Dupont R&D (USA) and Ames Lab (Iowa, USA) before joining IIT Delhi in 1995. His main interest is in the area of design of new materials, especially nanomaterials for energy conversion and superconducting materials. He has published over 350 papers and has filed five patents (two granted).

He is a recipient of the MRSI Medal, CRSI Silver & Bronze Medal & CRSI-CNR Rao National Prize, National Award of Nano Science and Nanotechnology (DST Govt. of India), Bangalore India Nano award (Karnataka Govt) and Distinguished Materials Scientist of the Year Award (2021), by the Materials Research Society of India, A V Rama Rao lecture Award and J N Mukherjee lecture award (Indian Chemical society). He is a fellow of the Indian National Science Academy, Indian Academy of Sciences and the National Academy of Sciences (India), Royal Society of Chemistry (London) and the Asia-Pacific Association of Materials. Dr Ganguli was keenly involved in the formation of Delhi S&T Cluster (DRIIV) part of the initiative of PSA, Govt of India. Dr Ganguli has very keen interest to promote outreach activities for underprivileged sections of society and has been to remotest schools and colleges in several states in the country.

III-V Semiconductor Quantum Dots: Synthesis and Applications

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Colloidal semiconductor quantum dots (QDs) were discovered around 40 years ago and gave rise to the 2023 Nobel prize in Chemistry. They have attracted considerable interest due to their unique size-dependent optical and electronic properties. Most research has been conducted on binary cadmium- and lead-based QDs (CdSe, PbS, etc.), which cover the visible and near infrared spectral range and can be easily synthesized using colloidal chemistry. However, the toxicity of these compounds strongly limits their use in real-life applications. III-V QDs such as InP and InSb are promising alternatives,[1,2] even though little is known about their toxicity. Moreover, their more covalent character, high oxidation sensitivity and scarcity of appropriate group-V precursors makes it much more challenging to achieve a precise control of their size, shape and surface state, and hence of their application-relevant properties.

This presentation will focus on the most recent approaches in the synthetic chemistry of III-V QDs and of their core/shell structures in view of their use in various types of applications in life sciences and optoelectronics. I will also discuss the toxicity profile of InP-based QDs in their pristine state and under accelerated weathering conditions.

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Dr. Peter Reiss is Research Director at the Interdisciplinary Research Institute of Grenoble (IRIG), France, and Deputy Head of the SyMMES laboratory, which focuses on molecular systems and (nano)materials for energy and health. He graduated from University of Karlsruhe (Germany), and received his PhD in Inorganic Chemistry under the supervision of Prof. Dieter Fenske (2000). His research activities focus on colloidal semiconductor quantum dots and metal halide perovskite nanocrystals, in particular their synthesis, surface functionalization and assembly of these nanoscale building blocks into functional materials. The studied applications range from biosciences, LEDs and photodetectors to energy conversion and storage.
Dr. Reiss acts as associate editor for *Discover Nano* (formerly *Nanoscale Research Letters*), and is Editorial Board Member of *Scientific Reports* (NPG). He co-organizes the biennial conference NaNaX – Nanoscience with Nanocrystals (http://nanax.org), the most important European meeting in the field of colloidal nanocrystals.

Label-Free Single Molecule Sensing with Metamaterials

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Metamaterials, designed structures with sub-wavelength featured constituents, can be designed for specific applications. Plasmon-mediated local field enhancement to resonances in metamaterials was used for single molecule detection. A perfect absorber-based metamaterial with ellipsometric measurements of differential phase has been shown to have single molecule sensitivity. However, selectivity or label-free detection is still a challenge. Surface enhanced Raman scattering (SERS) could be a useful tool to get selectivity if the substrate has a broadband response. A perfect absorber metamaterial and a novel broadband SERS substrate will be presented for high sensitivity measurements especially for label-free single molecule detection.

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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-photon metrology including single-photon emitters, detectors, and detection methodologies. He has over 145 journal publications. He is a fellow of 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 and to the executive committees of Asia Pacific Metrology Program (APMP), Optical Society of India (OSI), Indian Laser Association (ILA), and IEEE Photonics Mumbai Chapter. He is also a member of the Asia Pacific Physics Conferences, Condensed Matter Physics section.

Pushing the Limits of Photochemical Upconversion

Timothy W. Schmidt

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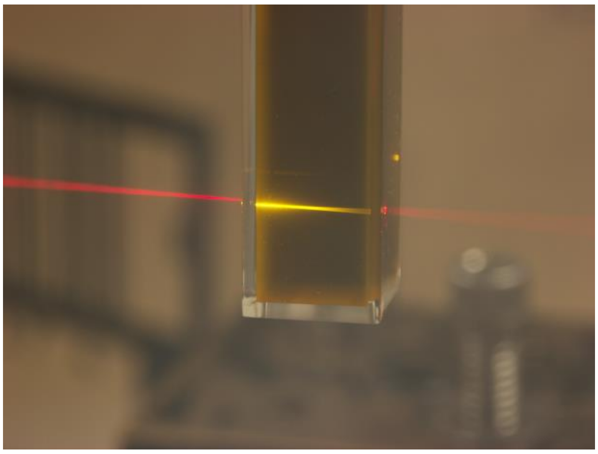
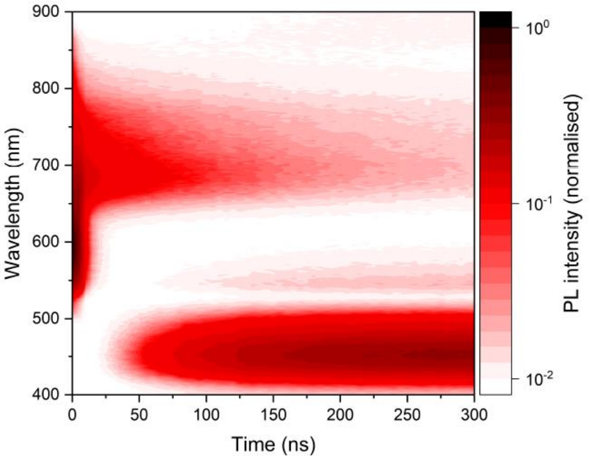
Photon upconversion using organic molecules is a promising phenomenon which could impact on a number of technologies including solar energy and fuels, photocatalysis, biological imaging and targeted drug release. The ultimate goal of this field is to convert lower energy photons into higher energy photons, as efficiently as possible in a convenient format. There are a number of challenges still to be overcome, including pushing the wavelength limits into the near infrared and the ultraviolet, and engineering solid state materials which efficiently upconverts under low levels of illumination.

In this talk I will discuss our approaches to upconversion from below the band gap of silicon,[1] and a surprising reversal of the role of oxygen at very low energies. I will also describe our recent approaches towards solid state upconversion devices harnessing nanostructured alumina scaffolds to sensitize upconversion in thin films.[2]





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Professor Timothy Schmidt was educated at The University of Sydney, winning the University Medal for Theoretical Chemistry in 1997. He undertook his PhD at The University of Cambridge in the field of femtosecond spectroscopy under the supervision of the late Dr Gareth Roberts. He was a postdoctoral research associate of Prof. Dr John Paul Maier, FRS in Basel, Switzerland, where he researched highly unsaturated hydrocarbon molecules of astrophysical relevance. Tim returned to Australia in 2003 to take up a position at CSIRO researching artificial photosynthesis. He was appointed as a lecturer in the School of Chemistry at The University of Sydney in 2004 and there rose to Associate Professor before moving to UNSW in 2014 as Professor and ARC Future Fellow. At UNSW he is Research Director of the School of Chemistry and Chief Investigator of the ARC Centre of Excellence in Exciton Science. Professor Schmidt has been the recipient of a number of awards for his research including the Coblentz Award (2010) for contributions to the science of molecular spectroscopy. He is a Fellow of the Royal Australian Chemical Institute, The Royal Society of Chemistry and the Royal Society of New South Wales.

Invited Lectures

Probing Local Surface Polarity of (Bio)molecular Aggregates using Sensitized Emission Imaging

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Forster resonance energy transfer (FRET) has been extensively used in the condensed phase to retrieve information on nanoscale proximity of different molecules/nanocrystals, and probe the transient interactions of bio-molecules or their fragments in solution. While FRET microscopy is routinely employed to detect interactions and conformational changes in biomolecules, such method becomes unreliable when the exact number of donor-acceptor (tagged) molecules are not known or if donor-acceptor pairs are not covalently attached to each other, such as that for self-assembled systems. In this talk, I will present a spectrally-resolved sensitized emission imaging method which allowed us to authenticate (bio)molecular interactions of donor-/acceptor molecules, given that sensitization of acceptor(s) mediated via energy transfer (from donors) decays rather sharply with distance and becomes negligible beyond several nanometers. I will discuss an application of this method to probe nanoscale surface polarity polymorphic biomolecular (amyloid) aggregates. The developed sensitized emission imaging method, which utilizes dual-color excitation coupled with multi-channel or spectrally-resolved imaging, can be used to study various luminescent self-assembled systems irrespective of their sizes, and becomes relevant to probe heterogeneity in parameters which are affected by nanoscale molecular interactions.

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) from Carnegie Mellon University. After a post-doctoral stint at Columbia University, Dr. Chowdhury joined IIT Bombay in 2006, where he established one of the first single-molecule fluorescence spectroscopy laboratories in India. His research focus has been to understand spatiotemporal heterogeneity in soft-materials, biophysics, semiconductor nanocrystals and perovskite crystals. He is also involved in the development of imaging methodologies and sensing analyte using living cells. Prof. Chowdhury is affiliated with the National Centre for Photovoltaic Research and Education (NCPRE), the Wadhwani Research Centre for Bioengineering (WRCB) and Sanghi Centre of Aging and Neurodegenerative Diseases (SCAN) at IIT Bombay.

1D Lead Halide Perovskites for Nonlinear Optics and Photonics

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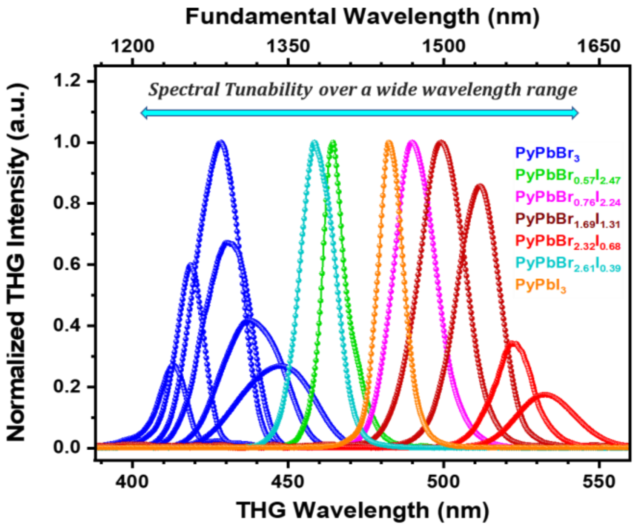
Nonlinear optics (NLO) is a great way to manipulate photon energies and has applications in photon energy upconversion, parametric amplification, photon detection, lasing and so on. However, there are only a handful of materials commercially available for NLO applications. Recently, the metal halide perovskites are in the forefront of research for their potential application in efficient photovoltaics, photocatalysis, and other optoelectronics. Motivated by the spectacular linear optical properties, we have explored the nonlinear optical properties of different low-dimensional metal halide perovskites. We observed excellent nonlinear efficiency and optical stability along with broadband tunability of NLO upconversion in these systems.



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Ph.D., Chemistry	Indian Institute of Science (IISc.), Bangalore, India Advisor: Prof. E. Arunan *Thesis Title: Rotational Spectra of Weakly Bound* H_2S *Complexes and 'Hydrogen Bond Radius'*	Sept 2005
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B.Sc. (H), Chemistry	University of Calcutta, Kolkata, India	July 1997

Details of positions held after highest degree:

Associate Professor	Department of Chemistry, Indian Institute of Science Education and Research (IISER), Pune, India	July 2017 – present
Assistant Professor	Department of Chemistry, IISER, Pune, India	Aug 2010 – June 2017
Postdoctoral Fellow	Rowland Institute at Harvard, Cambridge, MA, USA	Feb 2008 – Aug 2010
Postdoctoral Research Associate	Kansas State University Manhattan, KS, USA	Jan 2006 – Jan 2008

Surface-Ligand Interactions in Quantum Dots: 2D IR Insights

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The quantum dot surface plays a pivotal role as an interface connecting the semiconductor lattice and encapsulating ligands, significantly influencing the photophysical characteristics of semiconductor nanocrystals in various applications. Improving the conductivity and carrier mobility of nanocrystal-based devices can be achieved by substituting lengthy organic ligands with concise inorganic counterparts. However, a comprehensive understanding of the interplay between inorganic ligands and quantum dots remains challenging due to a lack of experimental methodologies directly investigating these ligands.

In my presentation, I will explore the outcomes of 2D IR spectroscopic investigations, shedding light on how variations in the dynamics of inorganic ligands provide insights into the diverse interactions between inorganic ligands and quantum dots. These results reveal discernible ligand dynamics time scales in quantum dots capped with SCN^- ligands as effective identifiers of distinct ligand populations, offering a molecular perspective on the intricacies of the quantum dot surface. Additionally, I will examine modifications in the presence of the electrical double layer in correlation with variations in quantum dot size.

In summary, my presentation aims to elucidate the application of 2D IR spectroscopy in unraveling these dynamics, providing a more comprehensive understanding of these interactions and opening avenues for novel applications and enhanced device performance.

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Bio-sketch

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Dr. Sayan Bagchi holds the position of Senior Principal Scientist in the Physical and Materials Chemistry Division at CSIR-NCL, Pune.
He earned his Ph.D. degree from the University of Pennsylvania (USA) in 2008. Following the completion of his Ph.D., Dr. Bagchi embarked on a post-doctoral research journey at Stanford University.
In 2012, Dr. Bagchi joined NCL as a Senior Scientist.

Within his laboratory, they conduct ultrafast two-dimensional IR experiments employing femtosecond pulses to capture spectral movies that illustrate molecular fluctuations. Dr. Bagchi's research interests encompass gaining spectroscopic insights into heterogeneous systems spanning the fields of chemistry, biology, and materials science. His approach involves a combination of experimental work and computational simulations to achieve a comprehensive molecular understanding of various chemical processes.

Light-Switches in Biomimetic Catalysis

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Light-powered molecular machines represent a remarkable class of nanoscale devices that uses the energy of photons to induce mechanical motion at the molecular level. Drawing inspiration from nature, these synthetic molecular machines emulate the functionalities of biological motors and enzymes. These machines consists of molecular switches that undergo conformational changes upon exposure to light. These switches serve as the impetus for precisely orchestrated movements of other molecular components, facilitating diverse functions, including rotary and linear motion, as well as the transport of cargo within the molecular domain. Furthermore, the judiciously planned orchestrated molecular motion can be used in regulating the activities of synthetic or biological catalysts.[1] This presentation will highlight a selection of light-driven molecular systems from our laboratory in which the occurrence of chemical reactions can be precisely controlled by light.[2]

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Subhajit Bandyopadhyay earned his Ph.D. from the University of Victoria, Canada. Following postdoctoral research stints at Columbia University and the University of Cambridge, he became an assistant professor at IISER Kolkata, where he presently a Professor. His academic pursuits span the synthesis and exploration of photochromic systems, the development of optical sensors for biologically significant analytes, machine learning applications, photo-controlled catalysis, and 'smartphone chemistry.' He is a fellow of the Royal Society for Chemistry and was selected for a DAAD fellowship and a joint INSA-Austalian Academy of Sciences fellowship. Beyond his scientific interests, he is a history enthusiast, and engages in painting.

Diindolocarbazole-Based Twisted Organic TADF Triads and Donor-Acceptor Compounds for Efficient Energy- and Electron-Transfer Photocatalysis

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Thermally activated delayed fluorescence (TADF) materials have received great attention because of their tremendous performance in organic light-emitting diodes (OLEDs).[1] For the achievement of high external quantum efficiency (EQE), the energy gap (ΔE_{ST}) between singlet state and triplet states should be small and photoluminescence quantum yields (PLQY) should be high.[2] Due to the long delayed lifetime and efficient triplet energy levels, TADF compounds have attracted great attention as photocatalysts for organic transformations over conventional metalated photocatalysts.[2] The talk will present organic TADF molecules **DI-IQ**, **DI-2FIQ** and **DI-PF** consisting of diindolocarbazole (DI) as electron donor and indoloquinoxaline (IQ), difluoro-substituted indoloquinoxaline (2FIQ) and fluorine substituted dibenzophenazine (PF) as electron acceptors.[3,4] Transient photoluminescence decay profiles of **DI-IQ**, **DI-2FIQ** and **DI-PF** indicate shorter prompt component and longer delayed component confirming the TADF nature of all molecules. Accordingly, these compounds were employed for E to Z isomerization of stilbene with maximum of ~78% conversion based on their triplet energy levels and in C-H arylation of various heteroarenes with excellent isolated yields of up to ~86%.[3,4] The talk will conclude with utilization of donor-acceptor (D-A) compounds for metal-free condensation cyclization reactions of aromatic aldehydes and *o*-phenylenediamine[5] as well as utilizing perylene derivatives-*g*-C_3N_4 composites for heterogeneous photocatalytic hydrogen evolution[6] and oxidative amidation reactions.

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Dr. Sanchita Sengupta received her M.Sc. Chemistry from IIT Kanpur and Ph.D. in organic supramolecular chemistry from University of Würzburg, Germany. Followed by a postdoctoral stay at Technical University of Delft, the Netherlands and an INSPIRE faculty fellowship at Indian Institute of Science (IISc), Bangalore, she joined IISER Mohali in the Department of Chemical Sciences in 2017 as an Assistant Professor and is an Associate Professor since Dec 2023. At IISER Mohali, her research interests include development of organic twisted donor-acceptor systems for photophysical phenomena such as twisted intramolecular charge transfer and thermally activated delayed fluorescence and their eventual applications in fluorescence ratiometric sensing, optoelectronics and photocatalysis. Further research directions of her group include development of multichromophoric energy transfer antenna and macrocyclic systems as multifunctional sensors and as materials for photocatalysis. Dr. Sengupta serves as a member in the Early Career Advisory Board of the journal ChemistrySelect. Dr. Sengupta was awarded the CRSI Young Scientists award in 2022, recipient of SERB POWER Grant (2022) and MoE-STARS Grant (2023).

From Molecule to Material: The Case of an Ultrashort Peptide

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Non-covalent interactions have been known for a long time and are used by supramolecular chemists to create soft materials of desired properties and applications. However, very frequently we encounter properties unknown to us, and in a way, supramolecular chemistry never fails to surprise us. This lecture comprises the story of an ultrashort peptide, PyKC.[1,2] The unusual self-assembly of the peptide to form a water-insoluble hydrogel and how the hydrogel opened up the possibility of creating new materials will be discussed. The unique confinement property of the hydrogel is used to trap and protect enzymes from external denaturants successfully for a long period. When combined with biopolymer, the hydrogel allowed us to create artificial synovial fluid for bone regeneration and cross-linker-free artificial cornea.[3,4] The thixotropic property of the hydrogel is further utilized to form stable macro-sized beads and hollow capsules.[5] The surface of the beads was decorated with AuNP and successfully utilized for catalytic purposes.

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Bio-sketch

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Debapratim completed his doctoral research under the guidance of Prof. P. K. Das from Indian Association for the Cultivation of Science, Kolkata, India. In 2007, he joined Prof. Herbert Waldmann at MPI Dortmund, Germany as an Alexander von Humboldt fellow. Thereafter, he moved to the University of Cambridge to work with Prof. Oren A. Scherman. In 2011, he joined the Department of Chemistry, Indian Institute of Technology Guwahati as an assistant professor. Since 2019, he has worked as a professor in the same department. Dr. Das' research focuses on supramolecular dynamic aggregates of peptide amphiphiles.

Styryl-Based Far-Red Emissive Fluorogenic Probes for Biological Applications

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Biomolecules such as proteins are dynamically active, incredible molecular machines in living systems to perform biochemical reactions.[1] Thus, their well-coordinated functions play a significant role in regulating various pathological and physiological disorders like inflammations, cancers, and neurodegenerative diseases.[2] Therefore, quantitative detection and real-time monitoring of biomolecules are important for pre-diagnosis and treatment of diseases.[3] In this regard, developing fast-responding reporter probes for sensing biomolecules holds great potential in biological applications.

We have developed 2-styrylchromone (**SC**) based far-red emissive probes for the detection of proteins and protein aggregates in aqueous media, biofluids, and animal models. Synthesized **SC** derivatives **SC1** and **SC2** potentially detected metabolic markers such as serum albumin in artificial urine samples (AUS) and blood samples. Also, achieved point-of-care detection of HSA by fabricating a cost-effective and portable test strip.[4] Furthermore, the mitochondrial targeting **SC1** identified the protein aggregates induced by lipid metabolites in live cells and *C. elegans*.[5] The biocompatible **SC-4mor** demonstrated the detection of protein inclusions in lysosomes, also in the neurodegenerative and non-degenerative models of drosophila.[6]

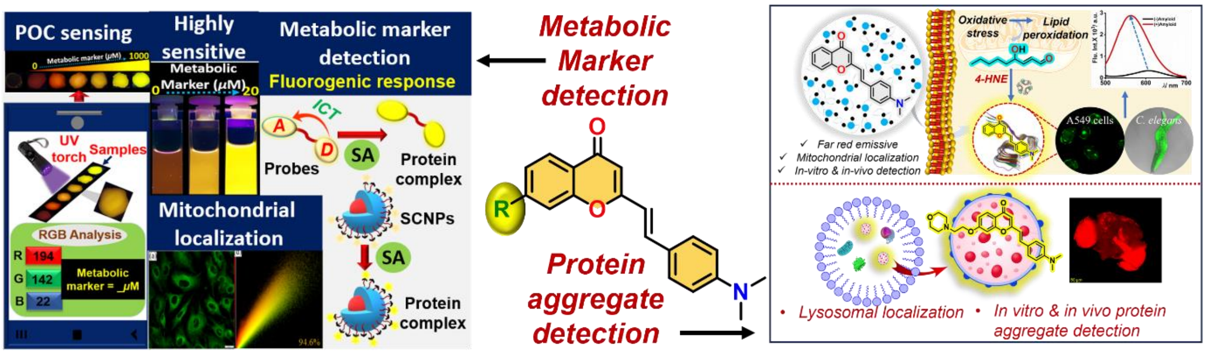

Figure 1. SC derivatives for detection of proteins and protein aggregates.

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Bio-sketch

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Dr. Koner is currently an associate professor at Indian Institute of Science Education and Research (IISER) Bhopal. He obtained his B.Sc. in Chemistry with the first rank in 2002 from Visva Bharati, Santiniketan. Then he moved to the Indian Institute of Technology Bombay (IITB) for master studies and worked on ultrafast excited-state processes in organized assemblies with Prof. Anindya Datta. After completion of his master's degree in chemistry from IITB, he went to Jacobs University, Germany and obtained second master's degree in Nanomolecular Science in 2006. Later in 2009, he received his doctoral degree from the same university on the topic of biomimetic supramolecular chemistry under the guidance of Prof. Werner M. Nau. He worked on diverse areas in physical organic chemistry. After completion of Ph.D., he started his postdoctoral work on nanobiotechnology at the University of Oxford as a Welcome Trust Postdoctoral Researcher from 2009-2010. In 2010, he received a prestigious Human Frontier Science (HFSP) Postdoctoral fellowship. So far, he has published over 110 research articles in international journals and guided 10 students for their Ph.D. and approximately 35 students for their master thesis. Currently, his lab is working on areas related to drug-delivery, physical organic chemistry, biophysics, chemical biology, and bio-nanotechnology.

Single Molecule Imaging through Engineered Molecular Interaction

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Fluorescence microscopy provides the most powerful tool for investigating biomolecules, particularly with the invention of diffraction-barrier-breaking super-resolution imaging techniques. Although existing super-resolution imaging techniques offer improved resolution, they require either complex and expensive instrumentation or specialized buffer conditions (buffers with reducing/oxidizing agents) along with high-power laser illumination to achieve optimal results. Additionally, the use of high laser power illumination and specialized buffer conditions to induce fluorescence blinking often limits the potential application of these techniques in live-cell imaging experiments. To address these challenges, we recently developed a simple, robust, and easy-to-implement single-molecule localization-based super-resolution imaging method using highly selective, strong, yet dynamic molecular interactions. Unlike existing techniques that rely on externally controlled ON- and OFF-blinking of fluorophores, our technique strategically exploits transient binding between molecular pairs to achieve autonomous blinking. By specifically targeting biomolecules in the living system, we have shown that this programmable and autonomous blinking with prescribed brightness and frequency enables two-dimensional (2D) and 3D super-resolution imaging of proteins in cells and tissues. Overall, our method offers an unprecedented level of resolution in a biological system without the need for complex instrumentation or specialized experimental conditions. I will delve into the intricacies of these strategies in detail during my talk.

Bio-sketch

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Dr. Sarit S Agasti is an associate professor at Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore. He obtained Ph.D. degree in Chemistry from the University of Massachusetts-Amherst. He worked under the guidance of Prof. Vincent M. Rotello. He joined Harvard University as a postdoctoral fellow, where he worked with Prof. Ralph Weissleder and Prof. Peng Yin. Dr. Sarit S Agasti is currently an associate professor at Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore. His research group focuses on the application of synthetic non-covalent recognition motifs, including host-guest interaction and DNA-DNA interaction, for developing new tools for biosensing, imaging, and therapeutic delivery. He is the recipient of the prestigious DBT/Wellcome Trust India Alliance Intermediate Fellowship, the Innovative Young Biotechnologist Award (IYBA), Sheikh Saqr Career Award Fellowship, Merck Young Scientist Award, INSA Medal for Young Scientists, the Asian and Oceanian Photochemistry Association (APA) Prize for Young Scientist. He also recently joined as an editorial advisory board member of the ACS journal Bioconjugate Chemistry.

Strategies and Challenges in Engineering the Excited State Processes of Fluorogenic Molecules

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Fluorogenic molecules have diverse potential applications, e.g. in fluorescence sensing and as solid state emitters. The key to control their light emitting properties is in the design of conditions that suppress nonradiative deactivation pathways of their excited states. Our attempts to do so with two classes of molecules will be discussed. The first is based on Dimethyl-2,5-bis(4- (methoxyphenyl) amino) terephthalate (DBMPT), which exhibits Aggregation Induced Enhancement in Emission (AIEE). This molecule exhibits strong fluorescence in its aggregates with surfactants[1] and triblock copolymers.[2] These aggregates form either nanorods or microspeheres and exhibit shape dependent cellular uptake. Their mixtures with appropriate blue emitters result in white light emission. Curiously, such white light emission with thioflavin T-containing amyloid fibils involves a disruption of the fibrils by the nanorods.[3] On a different note, ortho-substituted phenolic Schiff bases, which are very feebly fluorescent, exhibit a turn-on of fluorescence upon complexation with Zn^{2+} or Al^{3+}.[4-6] The extent of fluorescence enhancement is usually larger with Al^{3+} than with Zn^{2+} and π-stacking appears to hinder fluorescence. An interesting afterglow is obtained with adducts of one of these Schiff bases with boron. Hence, several aspects of the design of "to order" emission from this class of fluorogens is unveiled.

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2. Rakshit, S.; Das, S.; Govindraj, R.; Maini, R.; Kumar, A.; Datta, A. Morphological evolution of strongly fluorescent water soluble AIEEgen-triblock copolymer Mixed aggregates with shape–dependent cell permeability. *J. Phys. Chem. B* **2020**, *124*, 10282-10291.
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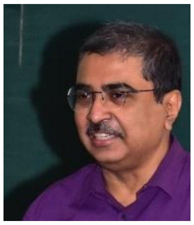

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Education

Ph. D.	Indian Association for the Cultivation of Science (Jadavpur University)	Picosecond laser spectroscopy	1998
M. Sc.	University of Calcutta	Chemistry, (Specialization in Physical Chemistry)	1994
B. Sc.	Presidency College, University of Calcutta	Chemistry (Honours), Physics, Mathematics, English	1992

Experience

Professor	Department of Chemistry, Indian Institute of Technology Bombay	2012–
Associate Professor		2007–2012
Assistant Professor		2002-2007
Visiting Scientist	Raja Ramanna Centre for Advanced Technology, Indore, India	2000–2002
Postdoctoral Researcher	Iowa State University, USA	1998–2000
Lecturer	Raidighi College, India	1997–1998

Administration

Head, Department of Chemistry	IIT Bombay	2018-2021
Head, Center for Research on Naotechnology and Center for Sophisticated Analytical Instrumental Facility (CRNTS-SAIF)		2016–2018
Associate Dean (Student Affairs)		2013–2015

Awards and Recognition

Bronze Medal	Chemical Research Society of India	2018
Fellow	National Academy of Sciences, India	2017
Award for Excellence in Teaching	IIT Bombay	2017
G. V. Bakore Memorial Award	Indian Chemical Society	2011
Young Researcher Award	Chemical Research Society of India	2006
Young Investigator Award	IIT Bombay	2005

Guidance of Ph. D. students
21 students have obtained Ph. D. 6 are presently enrolled.

Other responsibilities

- Guest Editor for Kankan Bhattacharyya Festschrift, J. Phys. Chem. B 2021
- Guest Editor for Institute Highlight on IIT Bombay. Joint Special Issue of ChemPhysChem, Eur. J. Inorg, Chem. and Eur. J. Org. Chem. 2020
- Member, Editorial Advisory Board, J. Phys. Chem. 2020-2022
- Vice President, Indian Laser Association, 2019-2023
- Treasurer, Fluorescence Society of India, 2012 onwards
- Mentor, Indian Team for International Chemistry Olympiad, 2015-2016

Time-Domain Broadband Circular Dichroism Spectroscopy: A Novel Probe of Chiral Structure and Spin Dynamics

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Among different spectroscopic methods, circular dichroism spectroscopy stands out for its unique sensitivity to chiral-optical and magneto-optical properties through light polarization. This makes ultrafast circular dichroism spectroscopy an ideal technique to probe photoinduced chiral structures and spin depolarization dynamics in biomolecular and material systems. The measurements remain challenging, however, due to the extremely weak nature of chiral light-matter interactions and significant polarization-induced artefacts. In this talk, I will discuss our recent effort on the development of time-domain broadband circular dichroism spectroscopy as a unique tool to probe chiral structure and dynamics. In particular, I will highlight the development of an optical setup capable of simultaneously measuring broadband circular dichroism (CD) and optical rotatory dispersion (ORD) spectra with high sensitivity. Different from standard approaches based on polarization modulation, the setup combines common-path polarization division interferometry with heterodyne time-domain balance detection to fully resolve the chiral signal field in its amplitude and phase. The setup accepts broadband ultrashort pulses and lays the foundation for high sensitivity probing of photoinduced chirality and spin with femtosecond time resolution. I will conclude the talk by outlining our ongoing effort to address unsolved problems on chirality using the broadband femtosecond circular dichroism spectroscopy technique.

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Bio-sketch

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Soumen Ghosh is an Assistant Professor at the Department of Inorganic and Physical Chemistry in Indian Institute of Science (IISc), Bangalore. He obtained M.Sc. in Chemistry from IIT Kanpur. Soumen completed his PhD in Chemistry at Michigan State University, USA under the supervision of Professor Warren F. Beck in 2017. Subsequently, he moved to Politecnico di Milano, Italy as a Marie-Curie/Postdoctoral Fellow in the group of Professor Giulio Cerullo and Professor Dario Polli. After finishing his postdoc, Soumen joined the Indian Institute of Science (IISc) Bangalore as an Assistant Professor in November 2022. His research group at IISc are currently focused on the development and applications of chirality-sensitive femtosecond circular dichroism spectroscopy.

Symmetry Breaking Charge Separation in Chromophoric Dimers

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The independent discovery of dye aggregate by Jelley and Scheibe marked the beginning of a spectacular development in the field of aggregate photophysics.[1] Subsequent research warranted an exceptional model for defining the exciton interactions in aggregates, proposed by Kasha and Davydov independently, which was later modified by incorporating the short-range excitonic coupling.[2,3] Apart from the well-studied H- and J-aggregate, achieving the orthogonally cross-stacked assembly possessing null excitonic interactions remained elusive. The first crystalline evidence for the chromophoric Greek cross (+) assembly exhibiting monomer-like optical properties was reported in 2018 (Figure 1).[4] The emergent photophysical properties of the crafted Greek cross (+) architectures were explored using both experimental and computational techniques for understanding the aggregate properties beyond Kasha's model.[5,6] The manifestation of selective hole transfer coupling in the edge-to-edge arranged Greek cross (+) perylenediimide (PDI) dimer resulted in ultrafast dissociation of null exciton and evolution of the charge-separated state in a polar solvent, providing a way forward in the fundamental understanding of null aggregates.[7]

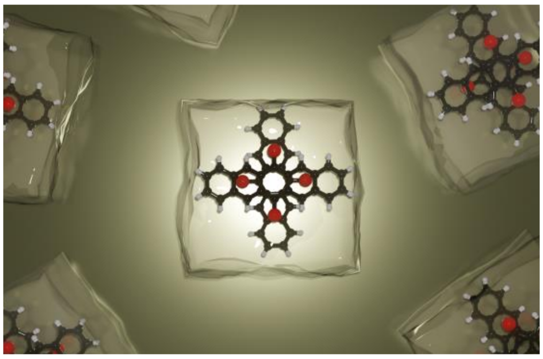

Figure 1. Schematic diagram showing the Greek-Cross aggregate.

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Tracking Correlated Triplet-Triplet Pairs in Singlet Exciton Fission

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Singlet fission[1-2] (SF) is a process by which an excited molecular chromophore in its singlet state shares its excitation energy with an unexcited proximal neighbour leading to formation of two triplet excitons through a spin-allowed process. Due to the high singlet-to-triplet conversion quantum efficiencies up to 200%, SF chromophores have potential application in boosting solar cell efficiencies beyond the Shockley-Queisser limit.[3] However molecular triplet excitons produced through SF usually have shorter triplet lifetimes due to exciton-exciton recombination and relaxation pathways, thereby resulting in complex devicearchitectures for SF-boosted solar cells. In order to elucidate the fundamental mechanism of SF and the triplet-triplet recombination pathways it is essential to understand the intrinsic electronic nature of the intermediate correlated T-T pair states delocalized over the two chromohores. In this talk, I will demonstrate through our work that coupling the chromophores in optimal morphologies/geometries allow for efficient SF as well as an unequivocal detection of the correlated T-T pair state.[4-7] At the end, I will touch upon the significance of understanding the T-T pair state in enabling a testable structure-function relationship for next generation SF-boosted solar cells.

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Prof. Jyotishman Dasgupta received his 5-years Integrated Master's 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 currently as a Professor. 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 Young Scientist Award from the Asian and Oceanian Photochemical Association (APA), 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: *JPC Letters*, *Journal Physical Chemistry* and *Journal of Chemical Physics*.

Engineered Solid-State Aggregates in Brickwork Stacks of *n*-type Organic Semiconductors: A Way to Achieve High Electron Mobility

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Economic and synthetically viable *n*-type organic semiconductor materials and solution-processed OFET devices with ambient stability and high electron mobility are rare. Converging all these desired requirements into a single molecule is still challenging; at the same, it is the need of the hour. Synthetic viability (less than three steps) and cost-effective starting materials are essential to achieve the same. Here, we discuss our strategy to achieve the right candidate with the above criteria. Napthalenedimiide (NDI) core structures were identified and we are revisiting the core- substitution strategy of the n-type planar aromatic core by easy synthetic route (two steps with 70% synthetic yield and 7 \$/g material cost). The key highlights such as the solution-processed OFET devices with appealing electron mobility in the bulk film state (> 1 $cm^2V^{-1}sec^{-1}$ with an on-off current ratio of 10^8) and ambient stability. A detailed investigation of the need for the unique supramolecular arrangement of the outperforming material in its Brickwork stack was systematically conducted and compared with two structurally similar model derivatives to assert our claims. Interlocked charge hoping units of the NDI core units in their Brickwork stack in the former case were found to be the principal reason for the superior device performance. Detailed electronic, spectroscopic and microscopic studies of the layers will be discussed.

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2	Asst. Professor (On Contract)	IISER Kolkata	July 2015	January 2016
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Emerging Polarized Light Methodologies for Probing Nano Scale Structural Anisotropy

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In this talk I shall introduce some new experimental concepts of polarimetry for probing structural anisotropy of biological tissues and other complex materials at the nanometer (sub-wavelength) length scales. Specifically, a custom designed state-of-the-art dark-field spectroscopic Mueller matrix microscopy system will be discussed, which has the ability to extract complete polarization information and to quantify the intrinsic polarimetry characteristics from even a single isolated nanoparticle / nanostructure. An illustrative example of the exceptional ability of this system will be presented, where this polarization microscopic system in combination with a suitable polarization analysis model enabled quantitative assessment and understanding of the self-healing behavior of a bio-inspired piezoelectric organic crystal by sensing changes in structural anisotropy in the nanometer length scale. A spectral Mueller matrix based inverse light scattering polarimetry method for the quantification of nanometer scale multifractal (multi-scale self-similar) anisotropy of tissue will be presented and its initial application for pre-cancer detection will be discussed.

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Nirmalya Ghosh is a physicist with specialization in optical physics and photonics. He joined Indian Institute of Science Education and Research (IISER) Kolkata, India in 2010 and is currently Professor in the Department of Physical Sciences and Centre of Excellence in Space Sciences India (CESSI), IISER Kolkata. At IISER Kolkata, he developed and runs bio-optics & Nano-photonics (bioNap) research laboratory. The group has made important contributions in areas of spin (polarization) optics, weak measurements, plasmonics and biophotonics. He is the recipient of the G. G. Stokes Award in Optical Polarization given by SPIE. He is also a Fellow of Indian Academy of Sciences and Fellow of National Academy of Sciences, India. He has authored over hundred papers in peer-reviewed international journals, and has also written several invited reviews, book chapters and a text book in the area of optical physics and photonics.

Electronic and Ionic Transport in Mixed Metal Perovskites

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Metal halide perovskites have exhibited outstanding device application, several fundamental questions related to the nature of the charge carriers, scattering mechanism, disorder dynamics etc. Field effect transistors provide an appropriate platform for probing these fundamental issues. Investigation of the inherent field-driven charge transport behavior of 3D lead halide perovskites has largely remained a challenging task, owing primarily to undesirable ionic migration and dipolar disorder effects. In this talk, I will discuss strategies to overcome both these challenges and demonstrate that field-effect transistors (FETs) based on methylammonium-free, mixed-metal (Pb/Sn) perovskite compositions, do not suffer from ion migration effects as their pure Pb counterparts and reliably exhibit hysteresis free p-type transport with high mobility reaching 5.4 cm^2/Vs, ON/OFF ratio approaching 10^4 , and normalized channel conductance of 3 S/m. The reduced ion migration is also manifested in an activated temperature dependence of the field-effect mobility with low activation energy, which reflects shallow electronic defects Furthermore, we perform detailed lateral and vertical measurement to clearly distinguish the ionic and electronic transport in these materials. Interestingly, we observe that incorporation of Sn minimizes the lateral and vertical ionic transport thereby providing fundamental insights into the doping, defect and charge transport physics of mixed-metal halide perovskite semiconductors.

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Dr. Satyaprasad P Senanayak is an Assistant Professor of Nanoelectronics and Device Physics in the National Institute of Science Education at Research (NISER), Bhubaneswar. He did his research and 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 and Royal Society Alumni Fellowship. He is a Early career member of American Physical Society, European Material Research Society, Associate of Indian Academy of Sciences and Odisha Bigyan Academy. His current research at NISER addresses two focused areas: (a) Development of high performance perovskite optoelectronic devices; (b) Thermoelectric Devices.

Doping of Soft Semiconductors towards Stable and Efficient Optoelectronics

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Semiconductor materials based on conjugated organic materials and halide perovskite materials are driving the progress of low-cost optoelectronics. For broader applications, electronic doping of these materials is required. For organic materials, molecular and metal complex-based dopants are often used for electronic doping. However, high costs, low doping efficiency and stability issues associated with these dopants demand alternative approaches. Toward that end, we have developed different types of dopants for an extensive range of organic semiconductors. These dopants provide efficient and stable doping of organic transport layers used in perovskite devices. We also show the application of this new type of doping method in metal halide perovskite solar cells, organic thin-film transistors, and organic light-emitting diodes.

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Electronic Structure and Optical Properties of I-III-VI_2 Semiconductor Quantum Dots

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Electronic structure and optical properties of I-III-VI_2 semiconductor quantum dots will be discussed. We will show how the interplay of defects and unusual band edge structure leads these semiconductors to exhibit several anomalies such as temporal evolution of radiative rates. We will further describe significance and limitations of comparisons of these materials with doped quantum dots.

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Excited State Dynamics and their Role in Biosensing

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Spectroscopic properties of a molecular system, which are being extensively used for different applications, like energy harvesting, photonics, optoelectronics, etc. largely depend on the extent of dissipation of the absorbed photon energy to different decay channels. Thus, knowledge of the excited state dynamics of molecular systems is essential for their efficient use in different optical applications. Non-radiative decay of the excited state molecule through different channels is mainly responsible for the low efficiency in photonic applications. Thus, suppression of such non-radiative decay channels is very important. Modulating such a non-radiative decay channel using a chemical route is widely used to attain the prescribed spectroscopic properties of a class of molecular systems. Such a chemical route is quite cumbersome due to complicated synthetic procedures to be followed. Suppression of the non-radiative process by a physical mean is desired by all spectroscopists. In the present talk, we will discuss our contribution to modulating the non-radiative decay channels of molecular systems in their excited state molecular system using a physical method and their applications in biosensing.

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Research Experience:

- Ultrafast chemical dynamics in condensed phase using different time resolved techniques.
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Light-Matter Interactions at Nanoscale Leading to Chemical Changes

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The ability to move energy and electrons, under the influence of sunlight, in an efficient manner is one of the fundamental challenges in energy research. Our group is interested in designing principles based on the interplay of forces at the nanoscale to improve the optoelectronic properties of nanomaterials.[1] For instance, the potency of electrostatic forces was elegantly explored to demonstrate efficient light induced energy and electron transfer processes in quantum dots (QDs).[2] Further, a fine control over such interaction driven photophysical processes helped in the creation of high-contrast multicolour luminescent patterns from a single QD nanohybrid film.[3] Similar control over interparticle interactions helped in outplaying the ligand poisoning effect in various nanoparticle (NP) catalysed photochemical transformations.[4] By tuning the NP-reactant interaction, we were not only able to achieve efficient catalysis at low NP concentration, but also regulated the catalytic properties between completely 'ON' and 'OFF' states - rendering the same NP as a catalyst or a non-catalyst.[5] Our group is also interested in '*selectively*' channelizing the hot-charge carriers as well as the heat generated in plasmonic NPs, for fuelling important chemical and physical transformations. These advancements achieved in the light harvesting properties of nanomaterials will surely enable us to practise chemistry in a more sustainable fashion.

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Long-Range Energy Transfer in Strongly Coupled Systems

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Light-mater strong coupling offers a unique way to control material properties by reshuffling the energy levels of the associated system. Here, a molecular state is coupled to a confined photon, forming hybrid *polaritonic states*. These half-photon-half-matter quasi-Bosonic states show intriguing properties such as energy-momentum dispersion and collective behavior.[1] Here, a single photon can get coupled to an Avogadro number of molecules that generate a collective state with much more improved transport properties.[2] We used this concept for long-range energy transfer experiments in conventional donor-acceptor systems. Our experimental finding suggests that polaritonic states can efficiently transfer energy beyond Förster distances.[3] We are building an analytical model to study the exact mechanism and the nature of the energy transfer in strongly coupled systems.[4] I'll also compare our experimental findings to the recent developments in the field.

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Dr. Jino George received his Ph.D. in chiral plasmonics (2012) from CSIR-NIIST Thiruvananthapuram (with Prof. K. George Thomas). Later, he spent five years at the University of Strasbourg, France, as a post-doctoral fellow (with Prof. Thomas W. Ebbesen). There, he explored the effect of strong light-matter interaction on the chemical and physical properties of coupled molecules and materials. At IISER Mohali, his studies are focused on understanding the properties of hybrid light-matter states and their application in controlling chemical reaction rates. Currently, he is interested in studying the transport behavior of electromagnetically dressed 2D materials like graphenes and TMDs.

Concurrent Energy Capture and Storage - Route to Formation of Solar Batteries

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The ability to directly capture and store solar energy in an electrical form within a single structure is an intriguing concept and if feasible, could be an ideal approach to overcome the intermittency issue of solar energy. Recently, ionothermal-treated carbon nitride has shown this unique dual functionality. However, the current understanding of the distinctive material is minimal and as such, presented here are data that give insight into how the dual function can be viably modulated without in fact altering the structure. Importantly, it has been shown that there is redox behavior in ionic carbon nitrides thus providing impetus for battery-like storage capability. Furthermore, the work demonstrates that by simply altering either the ions or the pH of the electrolyte, both the potential and storage capability of the photo-excited electron can be augmented. The former can be modulated over ca. 700 mV and the latter can be increased 4 times when Na ions are replaced by K ions. This work provides insight into ionic carbon nitrides and their seminal properties that are thus far not been realized in other conventional semiconductors.

Bio-sketch

Deepa Khushalani

Materials Chemistry Research Group, Department of Chemical Sciences, Tata Institute of Fundamental Research (TIFR) Mumbai, Mumbai 400005, Maharashtra, India.

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Web: www.tifr.res.in/~khushalani

- 2004 to Present – Currently Professor in Materials Chemistry at TIFR
- 2001 to 2003 – Lecturer in Inorganic Chemistry, University of Kent at Canterbury, UK.
- 1998 to 2000 - Post Doctoral Researcher, University of Bristol, UK.
- Ph.D. Inorganic Chemistry (1997) University of Toronto, Canada
- B.Sc. Chemistry (1992, 1st Class Honors) University of British Columbia, Canada

- Research Area: D Khushalani is a Materials Chemist and her area of expertise involves synthesis, characterization and application of a variety of inorganic structures such that (1) the morphology, phase, and size are carefully manipulated so that there is precise control over homogeneity and compositional purity, (2) the ensuing materials are applied in areas exploiting alternate sources of clean energy involving photovolatics and energy storage devices. Her group also works on drug delivery devices, photocatalysis and electrocatalysis.

- CRSI Bronze Medal in Chemistry 2018
- DST (Nanomission) Young Career Award in Nanoscience and Technology 2016
- Fellow of Royal Society of Chemistry (FRSC)
- Chair of RSC West India Section
- Editorial Board Member of Scientific Reports
- Member of Indian Academy of Sciences – Women in Science Panel
- Member of Royal Society of Chemistry, UK – Inclusion and Diversity Committee

Other Activities: Extensively involved in Science Outreach. Actively promoted basic sciences within rural and economically deprived areas of India. Given several workshops/lectures and mentoring sessions.

Reduction of Sulfur Dioxide to Sulfur Monoxide by Ferrous Porphyrin

Abhishek Dey

School of Chemistry, Indian Association for the Cultivation of Science, 2A Raja SC Mullick Road, Kolkata 700032, West Bengal, India.

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The reduction of SO_2 to fixed forms of sulfur can address the growing concerns regarding its detrimental effect on health and the environment as well as enable its valorization into valuable chemicals. The naturally occurring heme enzyme sulfite reductase (SiR) is known to reduce SO_2 to H_2S and is an integral part of the global sulfur cycle. However, its action has not yet been mimicked in artificial systems outside of the protein matrix even after several decades of structural elucidation of the enzyme. While the coordination of SO_2 to transition metals is documented, its reduction using molecular catalysts has remained elusive. Herein reduction of SO_2 by iron(II) tetraphenylporphyrin is demonstrated. A combination of spectroscopic data backed up by theoretical calculations indicate that Fe^{II}TPP reduces SO_2 by $2e^-/2H^+$ to form an intermediate $[Fe^{III}-SO]^+$ species, also proposed for SiR, which releases SO. The SO obtained from the chemical reduction of SO_2 could be evidenced in the form of a cheletropic adduct of butadiene resulting in an organic sulfoxide. The reaction proceeds via formation of an initial intermediate which is characterized using EPR and resonance Raman spectroscopy. The presence of 2nd sphere residues that assist in proton transfer mimics the lysine and arginine residues present in the distal site of Sir and accelerates the reaction.

References:

1. *Angew. Chem. Int. Ed.* **2023**, *62*, e2022152.

Bio-sketch

Abhishek Dey

School of Chemistry, Indian Association for the Cultivation of Science, 2A Raja SC Mullick Road, Kolkata 700032, West Bengal, India.

email: icad@iacs.res.in, abbeyde@gmail.com

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Abhishek Dey has a background in electronic structure in inorganic chemistry. His research aims at emulating the reactivity of enzyme active sites in synthetic analogues using the geometric and electronic structure function relationships present in natural systems. His current area of interest includes multi-proton and multi-electron transformations that are key for clean energy and environment and development of new analytical techniques for interrogation and intuition driven innovations in electrocatalysis.

Education:

Aug 2001 – May 2007	**Stanford University** PhD, Chemistry Palo Alto, United States
Aug 1999 – Jun 2001	**Indian Institute of Technology Kanpur** M. Sc, Chemistry Kanpur, India
Aug 1996 – Jun 1999	**Presidency College, Kolkata** B. Sc., Chemistry Kolkata, Bengal, India

Honors and Awards:

- **Fellow**, The National Academy of Science, India, 2023
- **Fellow**, The Indian Academy of Sciences, Bangalore**,** 2023
- **James Hoeschele Award**, Asian Society of Biological Inorganic Chemistry, 2022
- **CRSI Bronze Medal**, Chemical Research Society of India, 2020
- **SERB-STAR**, Department of Science and Technology, 2020
- **SBIC Emerging Investigator Award**, Society of Biological Inorganic Chemistry, 2019
- **Rising Star of Asia Medal**, Federation of Asian Chemical Societies, 2019
- **SPP/ICPP Young Investigator Award**, Society of Porphyrins and Phthalocyanine, 2014
- **Young Associate**, Indian Academy of Science, Bangalore, 2010
- **Young Investigator Award**, ACS, Division of Inorganic Chemistry, 2007
- **Evelyn Laing McBain Stanford Graduate Student Fellowship**, 2005

Synergistic activities:

- **Associate Editor**, ACS Catalysis.
- Editorial Advisory Board Member of Journals
- Present**: Chemical Communications, Journal of Inorganic Biochemistry (JIB), Chemical Reviews, Chemical Society Reviews, Resonance, ACS Central Science**
- Past*: Inorganic Chemistry, Journal of Biological Inorganic Chemistry* (JBIC), *ACS Catalysis*,
- Member DST Proposal Assessment Committee for TARE, Inorganic and Physical Chemistry (co-opted), SUPRA, Mission Innovation IC-5, SC committee on oxygen
- Guest Editor Virtual Issue of Inorganic Chemistry, J. Am. Chem. Soc. And ACS Catal. *The way forward in Molecular Electrocatalysis* **2016**
- Guest Editor Special Issue *Dalton Transactions* Frontiers in spectroscopic techniques in inorganic chemistry, **2017**

Fluorescent Copper Nanoclusters: A Versatile Candidate for Understanding its Interactions with Biologically and Environmentally Important Analytes

Moloy Sarkar

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In recent years, research related to nanomaterials has emerged as one of the most cutting-edge and modish areas of scientific exploration.[1] Among these nanomaterials, metal nanoclusters (MNCs) have garnered significant attention from researchers due to their ultrasmall size (<2 nm), low toxicity, advantageous optical properties, and excellent water solubility. However, studies on the interactions of MNCs with important analytes are still in their infancy. Therefore, further investigations on the said aspects are very much essential. Understanding the behaviour of MNCs, both in the absence and presence of different analytes, is expected to provide valuable information not only to comprehend the fundamental mechanisms governing their actions but also to generate knowledge that can be applied to various MNC-mediated applications such as bio-analysis, bioimaging, nanomedicine, sensing, optoelectronics, catalysis, energy harvesting etc.

The core of my presentation will revolve around the some works based on the interaction of copper nanoclusters (CuNCs) with biologically and environmentally important analytes, highlighting their diverse roles in sensing, enzyme inhibition, and catalysis.[2-3] I will discuss how CuNCs can act as a nano-senor capable of selectively and sensitively detecting highly reactive oxidative species (hROS) and antioxidants in a single chemical entity. I will be discussing about the potential of CuNCs as an effective enzyme inhibitor on the activity modulation of α-Chymotrypsin and the associated interaction mechanism. Successively, surface ligand mediated catalytic reduction of nitroarenes to the corresponding aromatic amine using CuNCs as nanocatalyst will be discussed.

References:

1. Mahmoudi, M.; Lynch, I.; Ejtehadi, M. R.; Monopoli, M. P.; Bombelli, F. B.; Laurent, S. Protein−Nanoparticle Interactions: Opportunities and Challenges. *Chem. Rev.* **2011**, *111*, 5610-5637.
2. Akhuli, A.; Chakraborty, D.; Preeyanka, N.; Dora, A. S.; Sarkar, M. Copper Nanoclusters as an Effective Enzyme Inhibitor on the Activity Modulation of A-Chymotrypsin. *ACS Appl. Nano Mater.* **2023**, *6*, 4910-4924.
3. Akhuli, A.; Preeyanka, N.; Chakraborty, D.; Sarkar, M. Turn-Off Detection of Reactive Oxidative Species and Turn-on Detection of Antioxidants Using Fluorescent Copper Nanoclusters. *ACS Appl. Nano Mater.* **2022**, *5*, 5826-5837.

Bio-sketch

Moloy Sarkar

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Dr. Moloy Sarkar did his Ph.D from the University of Hyderabad in 2007. Between 2007-2008 he was working as Research Associate in the University of Hyderabad. He joined NISER in 2009. Currently he is working as associate professor in the school of Chemical Sciences, NISER Bhubaneswar. He has produced 7 Ph.D students and Published more than 75 research papers as an independent researcher. His research area includes, Room Temperature Ionic Liquids, Deep Eutectic Solvents, fluorescence Organic and inorganic Nanoparticles.

Young-Investigators' Flash Presentation

Breaching the Diffraction Limit in Single Molecule Fluorescence Detection using Zero-Mode Waveguide (ZMW) Nanostructures

Satyajit Patra
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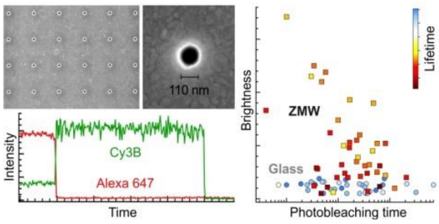
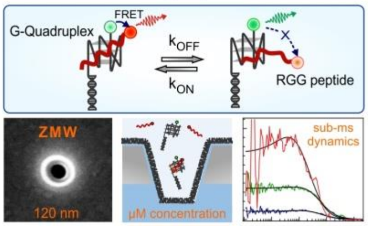
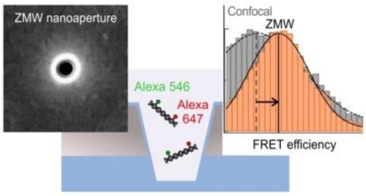
Due to a significant size mismatch between a single molecule and light wavelength, diffraction leads to a poor signal-to-noise ratio in single molecule measurements, impacting spatiotemporal resolution, and also restricts measurements to non-physiological nM-pM concentrations. In this context, metal nanostructures offer an elegant solution by localizing and concentrating light in the nanoscale far below the limit imposed by diffraction, utilizing localized surface plasmon resonance (LSPR). This enhances light-matter interaction, improving spatiotemporal resolution and enabling single molecule detection at physiologically relevant µM concentrations.

In my presentation, I will explore the utilization of aluminum nanoholes, also known as zero-mode waveguides (ZMWs), to overcome the diffraction limit in single molecule detection. The ZMW allows us to extend single molecule Förster Resonance Energy Transfer (smFRET) detection beyond the 10 nm limit with increased photon counts, leading to a significant enhancement in measurement resolution. Using ZMWs, we can conduct dual-color fluorescence cross-correlation spectroscopy (dcFCCS) studies at µM concentrations providing novel insights into the biomolecular interactions that necessitate µM concentrations. Moreover, ZMWs facilitate the attainment of a high photon budget for immobilized single molecules, enhancing the spatiotemporal resolution of these measurements. Overall, conducting single molecule measurements within ZMWs is crucial for advancing single molecule fluorescence spectroscopy.


Enhanced brightness for immobilized single molecule


Dual Color FCCS study at µM concentrations


Extend smFRET detection >10 nm

References:

1. Baibakov, M.; Patra, S.; Claude, J.-B.; Moreau, A.; Lumeau, J.; Wenger, J. Extending Single-Molecule Förster Resonance Energy Transfer (FRET) Range beyond 10 Nanometers in Zero-Mode Waveguides. *ACS Nano* **2019**, *13*, 8469–8480.
2. Patra, S.; Claude, J. B.; Naubron, J. V.; Wenger, J. Fast Interaction Dynamics of G-Quadruplex and RGG-Rich Peptides Unveiled in Zero-Mode Waveguides. *Nucleic Acids Res.* **2021**, *49*, 12348–12357.
3. Patra, S.; Claude, J. B.; Wenger, J. Fluorescence Brightness, Photostability, and Energy Transfer Enhancement of Immobilized Single Molecules in Zero-Mode Waveguide Nanoapertures. *ACS Photonics* **2022**, *9*, 2109–2118.

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Pilani, 333031, Rajasthan, India
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Research Interests

- Single molecule biophysics, nanoplasmonics, single molecule Förster resonance energy transfer (FRET), Fluorescence correlation spectroscopy (FCS) etc.

Professional Experiences

- **Jan 2022 – Present**: *Assistant Professor,* BITS-Pilani, Pilani campus, Rajasthan, India
- **July 2018 – Oct 2021**: ERC Postdoctoral Fellow, Institute Fresnel CNRS UMR7249, Marseille, France.
  Research Project: "*Breaching the diffraction limit in single molecule detection using nanophotonics*".
  Advisor: Prof. Jerome Wenger
- **July 2015 – June 2018**: Postdoctoral Reseracher, TU Dortmund & Ruhr University of Bochum, Germany
  Research Project: "*Exploring the crowding effect on DNA structure and dynamics*"
  Advisor: Prof. Roland Winter
- **Aug 2009 – May 2015**: Ph.D Researcher, University of Hyderabad, Hyderabad, India
  Thesis Title: "*Understanding the photophysics of quantum dots and diffusion of organic dyes in complex solvent media*".
  Advisor: Prof. Anunay Samanta

Total number of publications: 25, **Citations**: 942, **h-index**: 18, **i10-index**: 20

Source: Google Scholar

- 5 papers in journals with impact factor > 10 e.g. Angew. Chem. Int. Ed., Nucleic Acids Res., ACS Nano and Nano Lett.
- 20 papers in standard physical and biophysical chemistry journal with high visibility.

Ultrafast Intraband Spectroscopy of Perovskite Systems: Extending the Defect Tolerance to Hot Carrier Cooling Dynamics

Navendu Mondal

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'Defect-tolerant nature' of perovskites is under scrutiny due to the emerging reports of existence of surface defects in perovskite nanocrystals (NCs) to grain-boundaries in thin-films play crucial role in regulating the macroscopic performance like photoluminescence (PL) to device efficiency. Generally, the discussion around defect tolerance has focused largely on the recombination of band-edge (cold) carriers. Understanding the influence of these defects on hot carrier cooling (HCC) will also be critical for achieving more efficient NC-based devices but has not yet been thoroughly explored.

To address this knowledge-gap, we have studied HCC dynamics in $CsPbX_3$ (X=Br, I) systems of controlled defect density by employing pump-push-probe based optical spectroscopic measurements. The results reveal faster HCC dynamics for pure-Br, mixed-Br/I systems, with systematic increase in halide vacancies, contrastingly in pure-Iodide cases, HCC dynamics is independent to such defects. We believe halide vacancies induced trap-centres play a role in rapid trapping of energetic hot-carriers, while those trap-centres in $CsPbI_3$ are energetically much shallow in nature, thus having minimal impact on HCC. With the aid of kinetic modelling, we realize that saturation of trap-sites along with hot-phonon bottleneck effect at high HC density determine the HCC time for the halide-deficient systems.

Bio-sketch

Navendu Mondal

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London, London W12 0BZ, United Kingdom.

email: n.mondal@imperial.ac.uk

Navendu Mondal obtained his bachelor’s and master’s degree (with specialization in Physical Chemistry) in Chemistry from St Xavier’s College Kolkata (2010) and University of Calcutta (2012), respectively. He received his Ph.D. degree on the topic of ultrafast carrier dynamics in semiconductor nanosystems from School of Chemistry, University of Hyderabad in 2018. He has spent nearly 3-years of post-doctoral research at the physics department of the University of Texas at Dallas. Navendu moved to Imperial College London as a Marie Sklodowska-Curie Individual Fellow at the Ultrafast Optoelectronics Group of the Chemistry department in July 2021, currently he is extending his stay as Research Associate at the Imperial College London. His primary research interest lies in development of purpose-specific ultrafast optical-spectroscopic methods with both optical and electrical detection and apply them to optically control the structure-, charge- and energy- dynamics of functional semiconductor material systems at the nanoscale to tune their macroscopic properties.

Optically-Tracked Thermal-Breach-Memory in MaPbI$_3$

Kingshuk Mukhuti[a,b], Satyaki Kundu[a], Debasmita Pariari[c], Deepesh Kalauni[a], Ashutosh Mohanty[c], D. D. Sarma[c], Bhavtosh Bansal[a]

[a]Indian Institute of Science Education and Research Kolkata, Mohanpur, Nadia 741246, West Bengal, India.

[b]High Field Magnet Laboratory, Radboud University, 6525 ED Nijmegen, Netherlands.

[c]Solid State and Structural Chemistry Unit, Indian Institute of Science, Bengaluru 560012, Karnataka, India.

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Halide perovskite materials have been extensively studied in the last decade due to their impressive optoelectronic properties. However, their one characteristic that is uncommon for semiconductors is that many undergo thermally-induced structural phase transitions. The transition is hysteretic, with the hysteresis window marking the boundary of the metastable phase. We have discovered that in methylammonium lead iodide (MaPbI$_3$), this hysteretic metastable phase is athermal,[1] meaning it shows almost no temporal phase evolution under isothermal conditions.[2] Furthermore, under a reversible thermal perturbation, the states in the metastable phase either show return-point-memory or undergo a systematic irreversible phase evolution, depending on the thermal history and the sign of the temperature perturbation. Since the phase fraction can be probed via photoluminescence (PL), we have an optically retrievable memory that records any breach in temperature stability. Such thermal-breach-memory in athermal martensites, may be useful for tagging packages requiring strict temperature control during transportation or reservation.

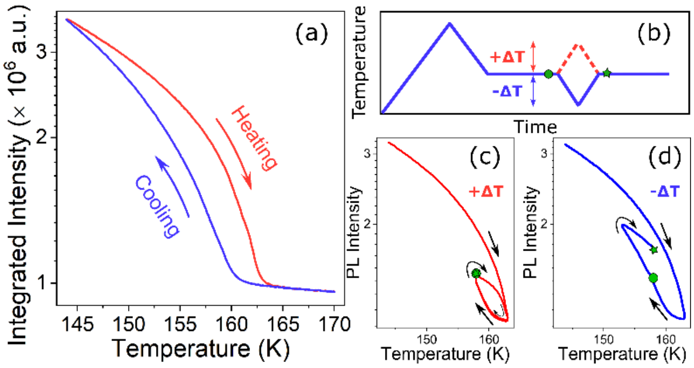

Figure 1. (a) Integrated PL intensity as a function of temperature for heating and cooling cycles. (b) Two states (green symbols) are created at the same temperature, but with different thermal history. (c, d) Integrated PL spectra show completely different intensity-evolution, depending on thermal history.

References:

1. Mukhuti, K.; Kundu, S.; Pariari, D.; Kalauni, D.; Mohanty, A.; Sarma, D. D.; Bansal, B. Evidence of Athermal Metastable Phase in a Halide Perovskite: Optically-Tracked Thermal-Breach-Memory. *Manuscript under review.*
2. Kundu, S.; Bar, T.; Nayak, R. K.; Bansal, B. Critical slowing down at the abrupt Mott transition: When the first-order phase transition becomes zeroth order and looks like second order. *Phys. Rev. Lett.* **2020**, *124*, 095703.

CONTACT INFORMATION

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RESEARCH AREA **Semiconductor Physics and Spectroscopy in High Magnetic Field**

EXPERTISE AND EXPERIENCE

For the last two years, I have been working on the transient emission spectroscopy of TIPS- Tetracene (single crystals), a well-known singlet fission system that has the potential to boost the solar cell efficiencies beyond the Shockley-Queisser limit. I have also been exploring phase transitions in iron-doped halide double perovskites through PL and Raman spectroscopy under steady magnetic fields upto 38 T. During my PhD, I mainly investigated the optical and magneto-optical spectroscopy of semiconductors and lanthanide-doped upconverting nanoparticles.

EDUCATION AND EMPLOYMENT

Postdoctoral Researcher December 2021 - present
Research Area: *Self-trapped excitons in halide double perovskites; Singlet fission processes in TIPS-tetracene crystals*
High Field Magnet Laboratory, Nijmegen, Netherlands

Graduate Student January 2016 - November 2021
PhD Thesis Title: *Optical and Magneto-Optical Spectroscopy of Semiconductors and Upcon- verting Nanoparticles*
Indian Institute of Science Education and Research Kolkata, India

Project Fellow 2012 - 2015
Topic: *Magneto-Dielectric Properties of Multiferroic Nanocomposites*
Supervisor: Dr. Pabitra Kumar
Chakrabarti The University of
Burdwan, India

M. Sc. Physics 2010 - 2012
Master's Thesis Title: *A Review of Magneto-Transport Properties and Magnetic Anisotropy in Granular Solids*
The University of Burdwan, India

The Mechanistic Insights into Drug Carrier Development, Cell Penetration Mechanisms, and Target Binding Studies

Anup Ghosh
DST Inspire Faculty
S N Bose National Centre for Basic Sciences, Kolkata 700106, West Bengal, India.
email: ghoshanup1603@gmail.com, anupg86@gmail.com

In recent years, functionalized nanomaterials have emerged as crucial components in modern medicine, serving as effective carriers for drug delivery to target cells. Our research has focused on investigating the surface-assembled structures of tri-peptide glutathione (GSH) on both silver (AgNP) and gold (AuNP) nanostructures, with a particular emphasis on their applications in biomedicine. We explored the surface chemistry and morphology of these nanostructures. Interestingly, we observed that GSH adopts a secondary structure on AgNP while exhibiting a random structure on AuNP. The choice of peptides is driven by their biocompatibility.

Concurrently, in our pursuit to comprehend the mechanism of cell membrane penetration, we investigated the structural and solvatochromic behavior of dimethyl sulfoxide (DMSO), a well-known cell membrane penetration enhancer. Surprisingly, our findings revealed that DMSO acts not only as a hydrogen bond acceptor but also as an effective acceptor through its α hydrogen atom. This discovery underscores the necessity for a reevaluation of the cell penetration mechanism, with the potential to pave the way for the development of superior cell penetration enhancers.

In our quest to unravel the structural information of proteins, peptides, and nucleosides engaged in hydrogen bond interactions with drug or ligand molecules, our work provides valuable insights. We specifically investigated the vibrational coupling of carbonyl (amide I) and the C=C transition of nucleobases. Our conclusions shed light on the intricate dynamics of coupled amide-I modes and highlight the dependence of vibrational coupling on various influencing factors. This knowledge holds promise for a more nuanced understanding of these interactions and their implications.

References:

1. Ghosh, A. Vibrational Coupling on Stepwise Hydrogen Bond Formation of Amide I. *J. Phys. Chem. B* **2019**, *123*, 7771-7776.
2. Chakrabarty, S.; Maity, S.; Darshana, Y.; Ghosh, A. Surface Directed Disparity in Self Assembled Structures of Small Peptide -L-Glutathione on Gold and Silver Nanoparticles. *Langmuir* **2020**, *36*, 11255−11261.
3. Chakrabarty, S.; Deshmukh, S.; Barman, A.; Bagchi, S.; Ghosh, A. On-Off Infrared Absorption of S=O Vibrational Probe of Dimethyl Sulfoxide. *J. Phys. Chem B* **2022**, *126*, 4501-4508.
4. Chakrabarty, S.; Barman, A.; Ghosh, A. Anomalous Infrared Absorbance of S=O/ C=O: A perturbation Study of α C-H/D *J. Phys. Chem. B,* **2022**, *126*, 5490-5496.
5. Chakrabarty, S.; Ghosh, A. Inconsistent Hydrogen Bond Mediated Vibrational Coupling of Amide I. *RSC Adv.* **2022**, *13*, 1295-1300.
6. Chakrabarty, S.; Barman, A.; Ghosh, A. A Disparity in Solvatochromism of C=O and S=O Vibrational Probe: A Study of Structurally Similar Acetone and Dimethyl Sulfoxide. *J. Mol. Liquids*, **2023**, *382*, 122005.

Dr. Anup Ghosh
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S N Bose National Centre for Basic Science
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Date of Birth: 16/03/1986

Academic Credentials

Research Experience:

- **DST INSPIRE FACULTY** – S N Bose National Centre for Basic Science, Kolkata [Working on Two dimensional Infrared Spectroscopy (2D IR) and small biomolecules].

  1st January 2019- continuing…

- **Postdoctoral Researcher** with Prof. Lev Chuntonov, Department of Chemistry, Technion-Israel Institute of Technology) [Worked on Two-dimensional Infrared Spectroscopy].

  2016 (May) - 2018 (December)

- **Postdoctoral Researcher** with Prof. Jyotirmayee Dash, Department of Organic Chemistry, Indian Association for the Cultivation of Sciences (IACS), Kolkata, India [Worked on structural determination of carbon dot].

  2015(August) - 2016 (May)

***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.

Master of Science (M.Sc., Chemistry, 2009), 1st Class, Department of Chemistry, Vidyasagar University.

Bachelor of Science (B.Sc., Chemistry, 2007), 1st Class, Vidyasagar University.

(10 + 2)th level, 2003, Science, 1st class, West Bengal, India.

10th level, 2001, Science, humanities, and language group. 1st Class, West Bengal, India.

Halide Driven Energy and/or Charge Transfer Dynamics in Perovskite Nanocomposite

Tushar Debnath

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Halide perovskite nanocrystals (PNCs) are gaining increasing attention in the contemporary research due to their unique physical properties and novel application possibilities like single-photon emitters for quantum technologies. We used a small bi-dentate molecule to surface functionalize $CsPbX_3$ PNCs (X= Cl, Br, I) to explore the surface coupling and their influence on the exciton/charge transfer dynamics.[1,2] The $CsPbX_3$ nanocomposite shows hydrogen bonding in the case of X=Cl and Br, that act as a charge transfer (CT) bridge for an ultrafast (~540 fs to 2 ps) hole transfer process. In contrast, a chelation is observed in the $CsPbI_3$ nanocomposite, without any active CT process. We further fabricate a type-II $CsPbX_3/CuInS_2$ heterostructure and investigate the energy transfer (ET) and CT dynamics via photoluminescence spectroscopy.[3] Considering the spectral overlap between $CsPbX_3$ donor and $CuInS_2$ acceptor, as well as thermodynamic energy level alignment, we shed light on the CT and ET processes in those heterostructures. Importantly, we find the driving force ($-\Delta G$) for the CT process follows X= Cl> Br> I in $CsPbX_3/CuInS_2$ heterostructure, though we observe the reverse order of the electron transfer process, for which we propose the electron transfer occurs in the Marcus inverted region. Our halide dependent controlled regulation of CT and/or ET processes in these nanocomposites may find promising optoelectronic applications.

References:

1. Manna, M.; Pal, S.; Bhandari, S.; Debnath, T. Halide Driven Halogen-Hydrogen Bonding versus Chelation in Perovskite Nanocrystals: A Concept of Charge Transfer Bridging. *J. Phys. Chem. Lett.* **2023**, *14*, 354–362.
2. Manna, M.; Debnath, T.; Bhandari, S. Chemical coupling of halide perovskite nanocrystals with metal quinolate complex for white light generation. *Chem. Commun.* **2023**, *59*, 1469-1472.
3. Shah, S. H.; Debnath, T. $CuInS_2$ Decorated Perovskite Nano-architecture: Halide-Driven Energy and Electron Transfer. (Submitted).

Bio-sketch

Tushar Debnath

Centre for Nanotechnology, Indian Institute of Technology Guwahati, Guwahati 781 039, Assam, India.

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Dr. Debnath is presently working as a principle investigator at the Centre for Nanotechnology, IIT Guwahati, India. 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 optical spectroscopy group leader at the department of physics, LMU from 2019 - 2022, and then he started his independent research group at IIT Guwahati, India (2022 - present). Dr. Debnath is an expert in the field of ultrafast spectroscopy. His research interest focuses on the investigation of the fundamental photophysics of semiconductor nanocrystal materials, primarily for energy-related applications. Dr. Debnath is the recipient of several national as well as international awards, including the Alexander von Humboldt fellowship, Germany (2018), and the Ramanujan fellowship, India (2022).

How Robust is Studying the Structural Dynamics of Biomolecules by Single Molecule FRET Spectroscopy?

Ganesh Agam

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Biomolecules function by small and large scale structural motions spanning over nanoseconds to seconds. Single molecule FRET (Foerster resonance energy transfer), is an established technique of single molecule fluorescence spectroscopy when combined with energy transfer between the fluorophores thereby measuring the nanometer distances between them[1]. Nanometer distance changes and their timescales generally relevant in biomolecules could be measured by single molecule FRET spectroscopy. Although, previous studies on variety of biomolecules, organic fluorophores, employed set-up configurations, and data analysis makes these experiments hard to compare.

Recent community wide single molecule FRET study measuring the nanometer distances between the organic fluorophores attached onto a double stranded oligonucleotides confirmed the robustness of this technique with high accuracy and precision[2]. To assess the consistency of the technique to measure the conformational dynamics on millisecond timescale in biomolecules, we measured the same protein samples together with the other 19 laboratories. The study reiterated the similar accuracy and precision in the nanometer distance measurements on proteins as on oligonucleotides. Furthermore, by identifying the potential variation inducing configurations in the measurement set-ups and avoiding the fluorophore induced effects, dynamic analysis on proteins proved to be reliable in distinguishing the millisecond timescales of sub-nanometer distance changes across the laboratories[3].

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Selected Publications

- Folding pathway of a two-domain discontinuous protein.
  Agam G, Barth A, Lamb DC. Minor revision in ***Nature communications*** 2023**.**
- Reliability and accuracy of single-molecule FRET studies for the characterization of structural dynamics and distances in proteins. ***Nature Methods*** 2023.
  Agam G*, Gebhardt C*, Popara M*, …, Lamb DC, Seidel C.A.M., Cordes T. (*shared first co-author)
- Determining the oligomeric state of proteins from Fluorescence anisotropy. ***Biophysical Journal*** 2020. Heckmeier PJ, **Agam G**, Teese MG, Hoyer M, Stehle R, Lamb DC, Langosch D
- Coordinated conformational processing of p53 by the Hsp70 and Hsp90 chaperones machineries. ***Molecular Cell*** 2019.
  Dahiya V, **Agam G**, Lawatscheck J, Rutz DA, Lamb DC, Buchner J.

Poster Presentations

HSA Sensing: A Tale of Two Probes

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Human Serum Albumin (HSA) is an important biomolecule owing to its diverse roles.[1] It significantly contributes to colloidal osmotic blood pressure and even mediates the transfer of ligands across organ-circulatory interfaces to vital organs. Fluctuating levels of HSA can, therefore, serve as an indicator for diverse diseases.[2] In this work, two serum albumin probes were designed based on donor-acceptor (NPNF) and donor-π-acceptor (A4) models. The probes were screened for selective sensing of HSA by steady-state fluorescence technique. Both probes exhibit twisted intramolecular charge transfer (TICT) behaviour and, therefore, show a turn-on emission in the presence of HSA. The limit of detection for NPNF was found to be 0.24 μM, whereas that of A4 was 1.36 nM. The study revealed that probe A4 bearing a D-π-A system is a better HSA probe due to its selectivity, sensitivity, response time, and emission wavelength.

Details of the work done will be presented in the poster during the conference.

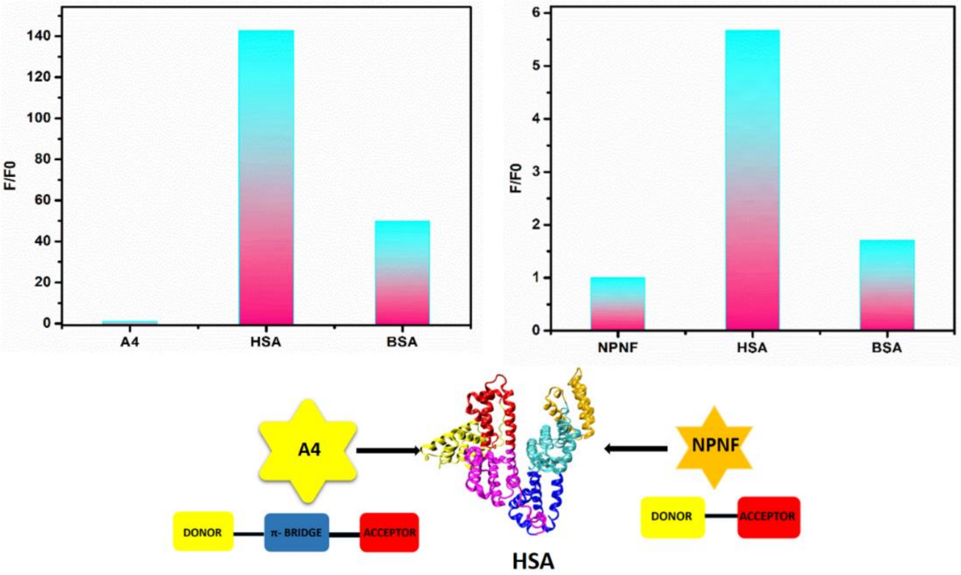

Figure 1. Comparative HSA sensing study of A4 and NPNF.

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Highly Selective Chromogenic and Fluorogenic Response of Pd^{2+} by using a AIE-Active Thiosemicarbazone Functionalized Pyrene Scaffold

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Herein, we have synthesised pyrene-linked naphthyl appended fluorogenic and chromogenic sensor $\mathbf{L_{A1}}$. The photophysical, as well as sensing behaviour of $\mathbf{L_{A1}}$, were examined by various spectroscopic techniques like UV-vis and fluorescence spectral analysis. $\mathbf{L_{A1}}$ displays a typical Aggregation Induced Emission (AIE) property (highly turn-on) in (3:7) MeOH/water mixture. Interestingly, the thin wire shaped nano-aggregates of $\mathbf{L_{A1}}$ were supported by FESEM and DLS analysis. The AIE-active probe $\mathbf{L_{A1}}$ specifically discriminate Pd^{2+} in presence of other competing metal ion via a colorimetric and fluorescence “turn-off” strategy through CHEQ mechanism. $\mathbf{L_{A1}}$ shows a detection limit (LOD) of 0.24 μM (25.46 ppb) with a binding stoichiometry of 1:1 with the guest analyte. DFT/TDDFT calculations were performed on $\mathbf{L_{A1}}$ and its metal complex to support the experimental outcomes. Additionally, the analytical performance of the chemoreceptor like on-spot detection of Pd^{2+} by TLC-based paper strips and detection of residual Pd in various active pharmaceutical drug ingredients are successfully implemented. Moreover, our synthesized probe $\mathbf{L_{A1}}$ also exhibited an anti-oxidant behaviour in presence of free radical DPPH.

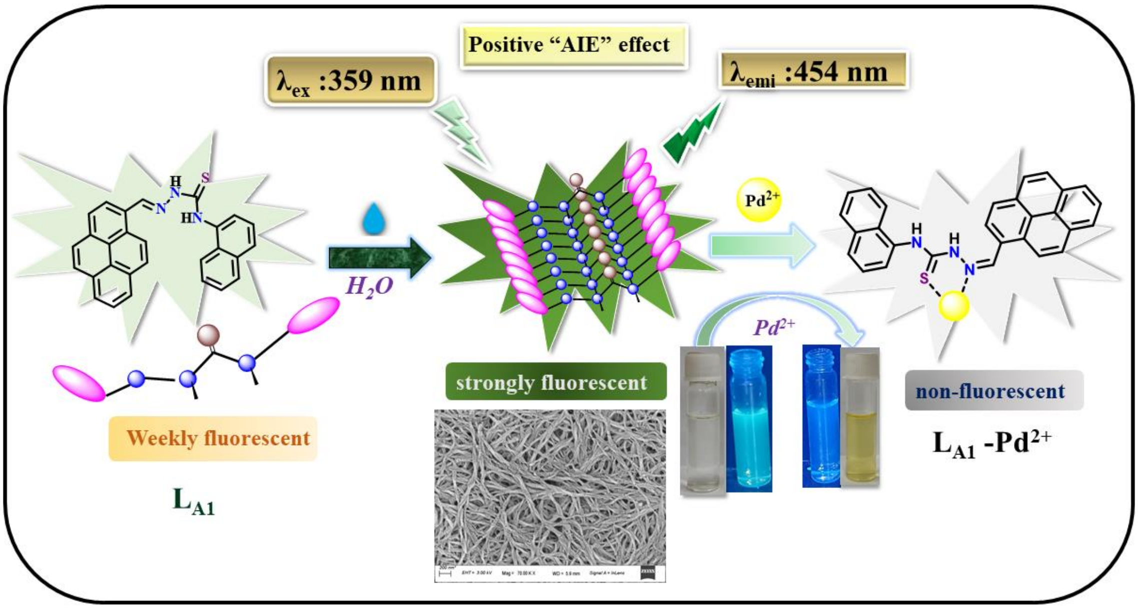

Figure 1. Graphical abstract.

Naphthalene Monoanhydride and Perylene Composites for Efficient Photocatalytic Hydrogen Evolution and Metal-Free Heterogeneous Oxidative Amidation

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Hydrogen is considered as one of the best candidates for solar energy storage that meets the growing clean energy demand and is one of the most important renewable energy sources.[1] Dye sensitization of graphitic carbon nitride (*g*-C_3N_4) is one of the most effective methods to prepare highly efficient photocatalyst with improved spectral response in the region above 450 nm.[2,3] In this work, we explored the synthesis of two visible light-active organic photosensitizer-based composites, naphthalene monoanhydride (Np) and 1,7-dibromoperylene monoanhydride diester (PMDE), with polymeric carbon nitride (*CN*) skeleton using calcination (c) and physisorption (a) methods. These composites showed enhancement of photocatalytic hydrogen evolution compared to only bulk-*CN* in water at neutral pH. Notably, **Np/*CN*(c)** achieves the highest hydrogen evolution rate (HER) at 1069 μmol $h^{-1}g^{-1}$, followed by **PMDE/*CN*(c)** at 705 μmol $h^{-1}g^{-1}$ and **Np/*CN*(a)** at 465 μmol $h^{-1}g^{-1}$. These rates represent significant improvements of 10, 7 and 4.8 times over bulk-*CN*/Pt respectively. These composite photocatalysts exhibited remarkable stability under prolonged photoirradiation, with hydrogen evolution consistently increasing with light exposure time. Additionally, these composites serve as efficient metal-free heterogeneous photocatalysts for the oxidative amidation of aromatic aldehydes with up to 80% product yields.

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An Insight into the Optoelectronic Behavior of Lead Halide Perovskite Quantum Dots with Tuned Composition

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The charge transport in semiconductor based optoelectronic devices is often driven by a facile interfacial transfer of charge carriers (electron/hole) on band-aligned inter-layer donor and acceptors[1, 2]. Enhanced charge transfer (CT) dynamics and collection of free carriers with reduced charge recombination are required for an improved performance[3]. Here, we explore the CT mechanism in $CsPbBr_3$ and the halide exchanged $CsPbCl_3$ perovskite quantum dots (PQDs) with two suitable small molecules as acceptors and its influence on their charge transport properties. The energy level alignment of these PQDs with respect to the HOMO-LUMO values of molecules is observed to be detrimental for the efficiency of photoinduced charge transfer and transport. The current conduction across an electrode-sample-electrode junction measured through conductive atomic force microscopy is found to be enhanced with acceptors. The conduction of charge carriers in these systems obeys tunneling mechanism exhibiting both direct and Fowler-Nordheim tunneling in the low and high bias regimes, respectively. The increased conductance is in agreement with the reduced barrier height across the junction. These findings can contribute to the development of efficient perovskite-based photovoltaics by employing simple, energetically suitable molecules as buffer layers between the active layer and charge transport layers.

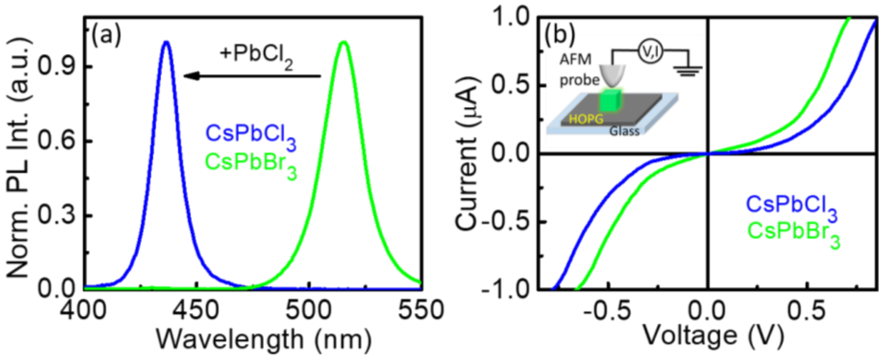

Figure 1. Normalized photoluminescence (PL) spectra (a) and current-voltage traces (b) of $CsPbCl_3$ (blue), $CsPbBr_3$ (green) PQDs. Inset of b illustrates the schematic representation of conductive atomic force microscopy measurement over a single PQD.

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Microviscosity-Assisted Disaggregation of a Model Ophthalmic Drug and FRET-Controlled Singlet Oxygen Generation in Lyotropic Liquid Crystals

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Different phases of lyotropic liquid crystals (LLCs), made up of mesogens like sodium dodecyl sulphate (SDS), mainly bestow different bulk viscosities. Along with that, the role of microviscosities of the individual LLC phases are of immense interest as a minute change in it due to guest incorporation can cause significant alteration in their property as potential energy transfer scaffold. Recently, the LLCs have been identified as plausible drug delivery agents for ocular treatments. In this direction, the present work illustrates photophysical modulations of an important laser dye as well as an ophthalmic medicine, Coumarin 6 (C6), inside different LLC phases in aqueous medium. C6 molecules spontaneously accumulate in water leading to aggregation caused quenching (ACQ) of fluorescence emission. However, the different phases of the LLCs prepared from SDS and water, helped in disintegrating the C6 colonies to various extents depending upon the microviscosities. This heterogeneity, in turn, could modulate the Förster resonance energy transfer (FRET) between C6 and N-doped carbon nanoparticles (N-CNP) incorporated inside the LLC phases. The N-CNPs acted as potential photosensitizers and generated singlet oxygen ($^1O_2$), a reactive oxygen species (ROS), to different extents. The microviscosities of the prepared LLCs were calculated, for the very first-time, using fluorescence correlation spectroscopy (FCS). The different phases of the LLCs, viz., lamellar and hexagonal, with different microviscosity affected the extent of C6 disaggregation, which, subsequently, controlled the FRET behavior and finally modulated the ROS generation. The results are encouraging since ROS generation plays a significant role in vision mechanism and LLC-based drug administration with potential FRET to control the ROS generation may become handy in ophthalmology. The LLC phases used in this experiment not only serve the purpose of drug delivery, but also the photophysical events therein are compatible to the ocular environment.

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Highly Stable Fluorescent $CsPbBr_3$ Perovskite Nanocrystals with Reduced In-Vitro Toxicity for Bioimaging and Mercury Ion Detection in Cells

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Recently, fluorescent $CsPbX_3$ (X = Cl, Br, I) perovskite nanocrystals (NCs) have been explored for the qualitative and quantitative measurements of heavy metal ions. The excellent multiphoton absorption property of the perovskite NCs also allows the integration of infrared light for fluorescent bioimaging applications. However, the poor structural stability of the perovskite materials against water, intense UV-irradiation, and leaching of Pb-ions into the environment remain great challenges for practical applications. In this regard, we encapsulated the $CsPbBr_3$ NCs with silicone dioxides (SiO_2) to improve NCs' stability while maintaining superior emission properties. These NCs were executed as a fluorescent probe for detecting mercury (Hg^{2+})-ions in water. Finally, these NCs were tested for sensing Hg^{2+}-ions inside the mammalian cells, demonstrating superior sensitivity for Hg^{2+}-ion detection.

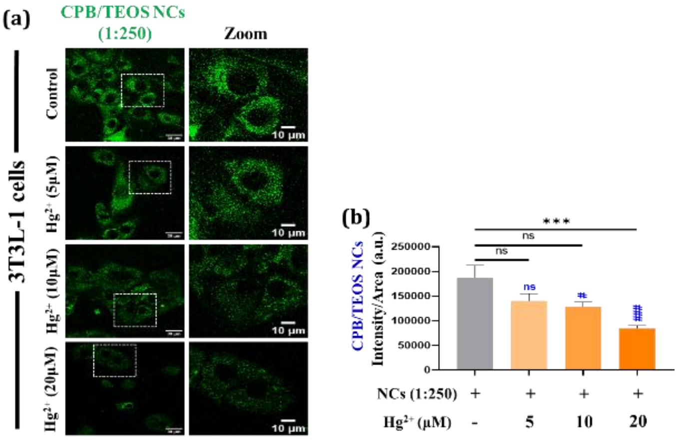

Figure 1. (a) Imaging of NCs treated living cells with increase in the Hg^{2+}-ions concentration, (b) Change in fluorescence intensity/area of NCs in cells with different concentrations.

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Tale of a Self-Sensitized Fluorophore: Towards Hypoxia Imaging and Photodynamic Therapy

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Molecular oxygen plays a crucial role in various physiological processes, but converting it to singlet oxygen leads to cell death. At the cellular level, deprivation of oxygen or hypoxia has been regarded as a salient feature of cancer. Thus, chemical probes that allow the in-depth investigation of biological hypoxia are important tools for understanding several diseases associated with low oxygen levels[1]. In type II photodynamic therapy, the photosensitizers generate singlet oxygen upon photo-irradiation. Therefore, our approach was to design a purely organic yet light-activable photo-sensitizer that can produce $^1O_2$. Herein, we have reported a metal-free dioxaborine-based fluorophore that undergoes self-sensitized photo-oxidation upon visible light irradiation in aerobic conditions accompanied by a change of fluorescence color from dark pink to pale green. The ratiometric changes in the emission intensity provide a quantitative estimation of the generated $^1O_2$. Moreover, we have extended our spectroscopic findings to live-cell imaging demonstrating the efficiency of our developed self-sensitizer to damage the cancer cells.

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Highly Efficient Color-Tunable Organic Co-Crystals Unveiling Polymorphism, Isomerism, Delayed Fluorescence for Optical Waveguides and Cell-Imaging

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Photofunctional co-crystal engineering strategies based on donor-acceptor π-conjugated system facilitates expedient molecular packing, consistent morphology, and switchable optical properties, conferring synergic ‘structure-property relationship’ for optoelectronic and biological functions. In this work, a series of organic co-crystals were formulated using a twisted aromatic hydrocarbon (TAH) donor and three diverse planar acceptors, resulting in color-tunable solid and aggregated state emission via variable packing and through-space charge-transfer interactions. While adjusting the strength of acceptors, a structural transformation into hybrid stacking modes ultimately results in color-specific polymorphs, a configurational cis-isomer with very high photoluminescence quantum yield. The cis-isomeric co-crystal exhibits triplet-harvesting thermally activated delayed fluorescence (TADF) characteristics, presenting a key discovery in hydrocarbon-based multicomponent systems. Further, 1D-microrod-shaped co-crystal acts as an efficient photon transducing optical waveguides, and their excellent dispersibility in water endows efficient cellular internalization with bright cell imaging performances. These salient approaches may open more avenues for the design and applications of TAH based co-crystals.

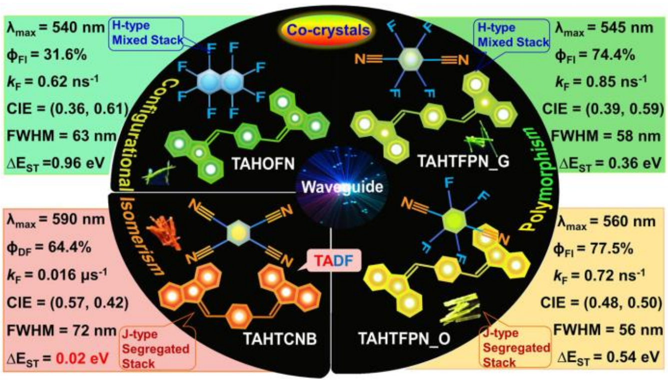

Figure 1. Graphical abstract.

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Photocatalytic Terminal C-C Coupling Reaction inside Water-Soluble Nanocages

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Natural enzymes carry out organic transformations via pre-organizing substrates inside hydrophobic cavities to achieve selectivity and specificity during reaction turnover. Chemists have mimicked the enzymes by creating supramolecular cavities which can serve as active sites for catalysis[1,2]. Recently it has been demonstrated that organic C-H activation reactions can be carried out inside a metal-based cationic water-soluble nanocage with visible light activation[3]. Here we aim to form C-C bonds via the donor-acceptor charge transfer (CT) paradigm. A Pd-based supramolecular cavity ($Pd_6L_4{}^{12+}$ where L= 2,4,6-Tri(4-pyridyl)-1,3,5-triazine) was used as host to encapsulate Phenylacetylene (PA) guest molecules . The host-guest complex was characterized by ^{1}H NMR and UV-Vis absorption spectra. Exciting at the CT band allow us the formation of C-C coupling products by coupling of two PA radicals via sequential electron and proton transfer steps. Characterization of photoproducts via GCMS and the mechanistic insights toward the formation of photoproducts had been investigated by EPR and time-resolved measurements[4].

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Controlling Dopant Photoluminescence in Samarium Doped Titanium Dioxide Nanoparticles by Subtle Alterations of Surface Capping Ligand

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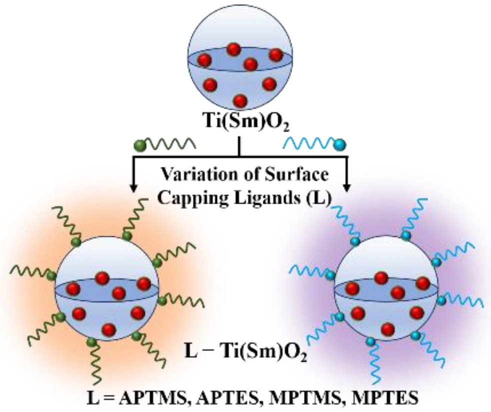
Surface of inorganic nanoparticles (NPs) in quantum confinement regime is extremely important due to high surface-to-volume ratio. Surface localized atoms and suitable surface capping ligands construct the surface. Trivalent lanthanide cation based luminophores are suitable for live-cell imaging, sensing, and light emitting diodes (LEDs) due to their non-overlapping sharp 4f-4f emission bands and longer luminescence lifetime. Our work systematically investigates the role of silane based surface capping ligand to control the dopant photoluminescence in trivalent samarium (Sm^{3+}) doped titanium dioxide NPs, with subtle alterations in their chemical structures. These molecules are (3-aminopropyl)trimethoxysilane (APTMS), (3-aminopropyl)triethoxysilane (APTES), (3-mercaptopropyl)trimethoxysilane (MPTMS), and (3-mercaptopropyl)triethoxysilane (MPTES). A remarkable change in rates of dopant emission depopulation is observed in Sm^{3+} emission lifetime measurements, whereas electronic structure of NPs is invariant that is guided by near constancy of NPs size. These results can primarily be well correlated with the environmental vibration of local environment, with a trend being more prominent in the case of more protected core sites. Signatures from Sm^{3+} located at the surface sites additionally compete with surface coverage by surface capping ligands. This work provides a foundation to help guide in choosing surface capping ligands for designing Sm^{3+} doped nanoparticles for biological applications.



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Light-to-Chemical Energy Conversion with Surface Engineered Quantum Dots

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Ability to play with the exotic photophysical and surface properties of quantum dots (QDs) have led the way of establishing the material as a potential photocatalyst in last two decades. Unlike molecular photocatalysts, QDs exhibit excellent size-tuneable core optoelectronic properties, along with rich and highly modular surface properties. The aim of our work is focused on developing a strategy to systematically modulating both the core optoelectronic as well as the surface ligand directed properties of the QDs to carry out a wide variety of chemical transformations under visible light.[1] Furthermore, efforts were made to investigate the stated objectives with environmentally friendly QDs (e.g. indium phosphide (InP) QDs), wherever possible, thereby enhancing the sustainability aspect of the QD photocatalysis. At first, the potency of InP/ZnS QDs was established in independently photocatalyzing two important classes of reactions, namely, metal-centred redox and organic C-C coupling reactions.[2] The two types of reactions were carried out in aqueous and organic medium respectively via proper surface engineering of the QDs. This work allowed us to reveal the full potential of the InP QDs in devising an artificial photosynthetic system via nicotinamide cofactor regeneration.[3] The photosynthetic light and dark cycles reactions were closely mimicked using our devised InP QD-enzyme nanobiohybrid system, which was finally applied for the continuous synthesis of useful chemicals under visible-light.[3] We could enhance the catalytic efficiency of the reaction by introducing favourable catalyst-reactant interaction via precise surface engineering of the InP QDs. In another attempt, the decisive role of ligand chemistry in directing the charge transfer process from the QD photocatalyst to the reactant was established. Here, we could identify and establish the dual role of triphenylphosphine in acting both as a surface passivating agent as well as a reactant in a series of QD photocatalyzed olefination reactions.[4]

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Engineering the Solid-State Aggregates in Brickwork Stacks of n-type Semiconductors by Structural Alteration: A Way to Achieve High Electron Mobility

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The studies and the great progress in the development of organic semiconductors (OSCs) have been constructed throughout the decades due to the vantages of being structurally designable, lightweight, low cost and mechanically flexible aspects towards the next-generation electronic devices like OFETs, solar cells, LED, sensors etc. As reliable electron-transporting *n*-type OSC materials are lagging behind *p*-type OSCs, and for the industrial advancement of OFETs, *p-n* heterojunction and integrated circuits assembled by both types of materials, the improvement of *n*-type OSCs including good environment stability and high electron mobility (μ_e) is in research hotspot.

Need of strong intermolecular interactions to minimize the longitudinal slip between π-stacked molecules and to reduce the lattice vibrations, special care is devoted to the molecular design strategy. Additionally, the substitution should favor effective solid-state aggregation which is crucial in achieving high μ_e and device stability, and also potentially lead to substantial electrostatic interactions in their aggregating solids states, particularly in the brickwork stack of molecular assemblies. Here, we achieved an n-type OSC with excellent dopant-free μ_e >1.0 $cm^2 V^{-1} s^{-1}$, and a very high I_{on}/I_{off} ($>10^8$) by solution process deposition. μ_e retained up to ~60 % upon ambient exposure for 100 h under 75 % humidity storage, indicating good ambient stability.

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Nanocrystals Embedded Organic Semiconductors for Field Effect Transistors

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Exploring and modulating intrinsic bulk and field effect charge transport of perovskite semiconductors has been a challenging task due to undesirable trap states, ion migration and associated dipolar disorder. We probe the charge transport physics of perovskite nanocrystals by understanding the different sources of traps and correlating the disorder with size of the nanocrystals, halide vacancies and role of the ligand moiety. Since these nano crystals do not exhibit a good field modulation due to the associated low conductivity of the ligands, we blend these NCs in bulk perovskite to demonstrate passivation of grain boundaries in 3D perovskite FETs and enhanced photoresponsivity in all perovskite phototransistors.

Role of the Tailored Hole Transport Layer in the Inverted Architecture Based Perovskite Solar Cells

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The inverted (*p-i-n)* architecture based perovskite solar cell is of significant interest due to low-temperature processed charge transport layers (CTLs). The energy band alignment between the charge transport layer and the perovskite absorber is essential for efficient photovoltaic performance. Perovskite is a class of material, and different compositions of perovskites can be prepared with different bandgaps (E_g) such as $FAPbI_3$ has $E_g \sim 1.5$ eV, $MAPbI_3$ has $E_g \sim 1.6$ eV, $CsPbI_3$ has $E_g \sim 1.7$ eV. Even changing the halides (Cl^-, Br^-, I^-) results in a change in the bandgap, especially the valence band. Therefore, the well matching band alignment of the hole transport layer (HTL) with different bandgap perovskites requires various kinds of hole transport layers of different HOMO levels. However, such complications of choosing different HOMO-level HTLs can be avoided by choosing a tailored HTL, i.e. mixing two molecules in different volume ratios. In this work, we used a self-assembled monolayer (Me-4PACz) and a conjugated polyelectrolyte polymer (PFN-Br), which have different work functions, and a mix of them in different volume ratios results in different work functions. Interestingly, a specific mixing composition (9:1) results in a well aligned work function of the mixed HTL with the 1.6 eV bandgap perovskite. We observed devices employing optimized Me-4PACz:PFN-Br (9:1) mixing ratio deliver open-circuit voltage (V_{OC}) of 1.16V and efficiency >20% for perovskites with a bandgap of 1.6 eV with high reproducibility and concomitant stability.[1]

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Comparative Anion Sensing Investigation using ESIPT Derivatives Featuring Unique Ring Expansions on the Proton Donor and Acceptor Sides

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Two derivatives utilizing the core structure of 2-(2’-hydroxyphenyl)benzimidazole, exhibiting ESIPT characteristics, were synthesized. One derivative, HNBI (D1), featured ring expansion on the proton donor side (hydroxyphenyl), while the other, HPNI (D2), showcased ring expansion on the proton acceptor side (benzimidazole). The study aimed to compare the sensing behavior of these derivatives with anions. Both D1 and D2 demonstrated swift responses with increased sensitivity towards CN^- and F^- ions by showing a shift in the absorption spectrum and fluorescence spectrum with enhanced fluorescence. Mechanistic insights into sensing were obtained through UV-Vis, Fluorescence, and NMR titrations, complemented by theoretical DFT calculations that concurred with experimental data. The detection limits for CN^- and F^- were determined as 6.8 nM and 4.5 nM respectively for D1, and 306 nM and 775 nM respectively for D2. Notably, the derivative with ring expansion on the donor side displayed lower LOD and superior sensitivity to CN^- and F^-. NMR and Fluorescence titrations unveiled a deprotonation mechanism leading to anion formation for D1 and D2. FESEM observations highlighted changes in the morphology of D1 and D2 after anion addition. Furthermore, the deprotonation mechanism was validated by introducing methanol as a proton donor, resulting in the fluorescence shift reverting to its original state. Consequently, D1 emerges as a promising candidate for extensive detection of toxic CN^- and F^- ions in the environment.

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Confined Two-Electron Hookium within DFT: Structure and Properties

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Atomic systems, when subject to external potentials, exhibit distinct features that offer valuable insights into their environments. The harmonium atom, serving as a simplified theoretical model in quantum mechanics, emerges as a crucial instrument for exploring the underlying principles governing electron behavior in two-electron systems. In this study, a density functional approach is proposed to investigate both ground and excited states of a two-electron atom confined within a harmonic potential.The radial Kohn-Sham (KS) equation is addressed using a physically motivated work-function based exchange potential[1], yielding results of nearly Hartree-Fock quality. Numerical accuracy is ensured through a generalized pseudospectral method (GPS) adhering to Dirichlet boundary conditions. Electron correlation effects are examined using a simple, parametrized local Wigner-type functional. Notably, the energy levels exhibit an increase in positivity with the growing strength of the confining potential. This research underscores the significance of the harmonium atom as both a pedagogical and conceptual tool, enriching our comprehension of quantum mechanics and electron correlation. With the advancement of refined models[2-3] and computational methods[4-6], the harmonium atom remains a pivotal resource in unraveling the intricate mysteries inherent in quantum systems.

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A Simple Ultrashort Fluorophore to Detect Cr (VI)

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In the era of urbanization, gradual accumulation of hazardous Cr (VI), in soil as well as water is a real concern to ecological health[1]. Bioaccumulation of Cr(VI) in the human body creates several life threatening diseases like renal and liver failure, haemolysis dermatitis, cancer etc[2-3]. So the detection of reactive Cr (VI) will be of great interests in the area of environmental as well as health related issues. Simple organic fluorophore based Cr (VI) sensors are rarely reported in literature. Herein we have reported a simple ultrashort fluorophore molecule which can selectively detect Cr (VI) over other metals ions. In presence of Cr (VI) the fluorescent intensity of the fluorophore diminishes whereas in presence of other metals ions the fluorescent intensity of the molecules enhances. Thus by showing an opposing spectral response towards Cr (VI) over other metals ions, the reported fluorophore can detect Cr (VI) in a unique way.

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Ensemble and Single Particle Photoluminescence of Quantum Dots in Plasmonic Field

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The undesirable trapping of photogenerated charge carriers in semiconductor quantum dots (QDs) to the mid-gap states detrimentally affects their brightness and color purity. The phenomenon of charge carrier trapping in QDs leads to trap state mediated photoluminescence (PL) and blinking. This inhibits the use of QDs as photon sources for various applications. While a plethora of chemical methods has already been devised to eliminate the trap states, these methods often involve tedious synthesis pathways.

Alternatively, modification in the photonic environment of the emitter can be achieved by physical methods[1] and the poster will demonstrate two examples of this concept. A physical approach for the selective enhancement of band edge PL of CdSe QDs over trap state PL by controlling the local photonic environment through the plasmonic coupling at the ensemble level will be presented in the first part. Frequency-specific plasmon resonance coupling selectively enhances the band edge PL and alters the spectral profile of the QDs.[2] The second example is based on single-particle investigations, wherein the intrinsic PL blinking of CdSe/CdS heteronanostructures is greatly suppressed by keeping them in the proximity of a plasmonic field.[3] A large increase in the radiative rate of the heteronanostructures along with their reduction in the Auger recombination significantly suppresses their blinking.

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Reconstructing Functional Protein from its Fragments

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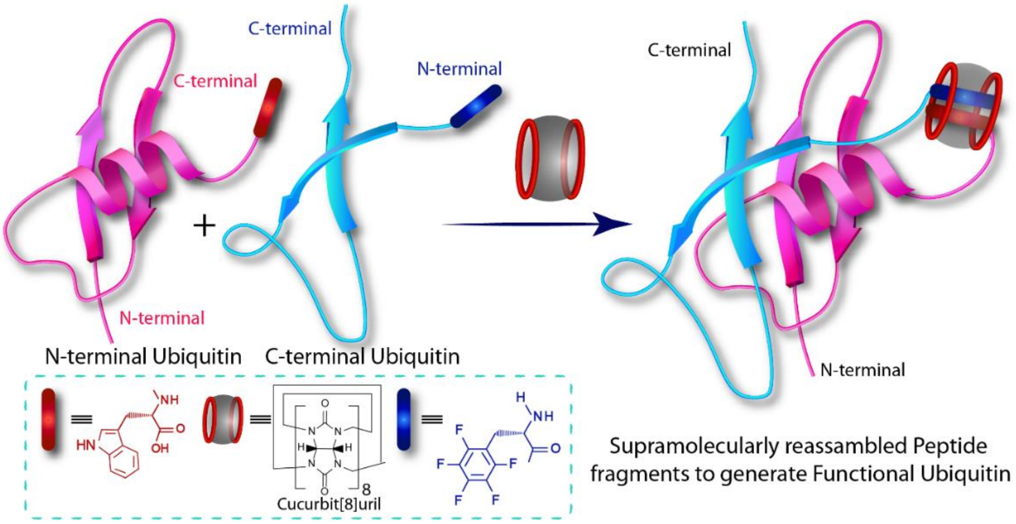
Control over protein function is highly desirable as it will allow us to understand and manipulate the biological phenomenon. In this regard, the Split-Protein Technique (SPT) provides unique opportunities where the fragments of a protein come into proximity and reconstruct the functional proteins.[1] The dissection and subsequent reassembly of a protein from its peptidic fragments allow control over its tertiary structure, and hence its function. In the present work, we utilized the host-guest chemistry of Cucurbit[8]uril (CB[8])[2] to develop a new strategy to reconstruct fully functional proteins from their peptidic fragments. As a proof of concept, two fragments of Ubiquitin are synthesized and functionalized with two guests for CB[8]. Under appropriate conditions, the guests form a ternary complex with CB[8], conjugating the two fragments. The conjugated protein showed similar folding to that of the native Ubiquitin. The activity assay confirmed that the reconstructed protein is fully functional. The observation opens up the possibility of using this newly developed split protein technique for various important biological applications.



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Understanding the Charge Transfer Mechanism in CsPbBr$_3$ Nanocrystals and Nitrogen-Doped Carbon Quantum Dots Heterostructures: Effect of Nanocrystals' Encapsulation

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Recently, lead halide perovskite nanocrystals (NCs) based heterostructures have demonstrated significant promise in various research areas, including solar cells, CO$_2$ reduction, and photocatalysis. These hybrid structures have also played a crucial role in advancing our fundamental conception of charge transfer mechanisms occurring at the interface. A thin shelling around the NCs is not suitable for the formation of stable and luminescent materials. So, understanding the mechanism of charge transport among the NCs dependent on the shelling materials is important. Here, we synthesized CsPbBr$_3$ NCs with various coating materials to vary the effective distance between the perovskite and nitrogen-doped carbon quantum dots (NCQDs) to understand the charge transfer process among them. So that we encapsulated the NCs with different coating materials such that the thickness of the NCs' shell can differ. We observed that the charge transfer rate between thick-shelled NCs and NCQDs is slow. The density functional theory (DFT) calculations of the heterostructure indicate that the electron acceptor state of the N-atom in NCQDs lies below the conduction band of perovskite NCs, which is accountable for such charge transfer. This study held immense significance as it provides crucial insights into the design and application of heterostructures.

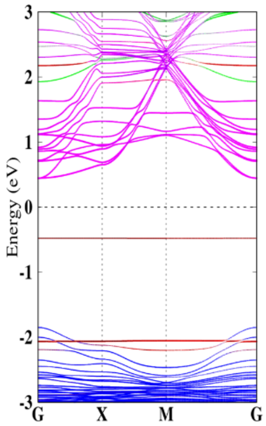

Figure 1. Projected band structures of NCQDs adsorbed on CsPbBr$_3$. (Cs: green, Pb: magenta, Br: blue, C: black, and N: red).

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Photoluminescent Crystalline Assemblies of Zn And Eu Mediated Gold Nanoclusters

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The systematic multicomponent assembly of atomic and molecular species enables the creation of superstructures with enhanced functionality. Investigating the effects of transition and lanthanide metal ions in self-assembling processes is both intriguing and vital for potential applications. This study explores the coordination of ligands stabilizing atomic nanoclusters with metal ions through complexation reactions, facilitating the development of higher-dimensional assemblies with novel optical and physical properties.

One notable achievement involves the fabrication of multi-layered two-dimensional (2D) nanosheets using dual-ligand stabilized gold nanoclusters (Au-NC) and Zn^{2+} metal ions.[1] These nanosheets exhibit an extended photoluminescent lifetime and show promise in energy storage at room temperature, efficiently storing molecular oxygen gas within the range of 0 to 20 bar at 20 °C.[1] Additionally, the study highlights the advantage of superior nanostructures over individual atomic Au-NCs, enhancing the prolonged emission of europium ions (Eu^{3+}).[2] Complexation with ligand-stabilized gold nanoclusters results in delayed fluorescence enhancement of Eu^{3+} ions, with selective augmentation in spectral lines attributed to $^5D_0 \rightarrow {}^7F_J$ transitions. The assembled crystalline structure of europium-containing Au NCs is confirmed through electron diffraction and high-resolution transmission electron microscopy analyses. This innovative design opens avenues for developing optical systems by combining molecular nanoclusters and atomic luminescent probes, presenting potential applications in various fields.

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Naphthalene Derived Hyper-Branched Polymeric Self-Assembly for Investigating Azoreductage Activity under Hypoxic Environment

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The design and synthesis of macromolecules through the introduction of controlled branching via hyperbranch polymerization gained recent attention of the scientific community due to its diverse application in the biomedical field starting from diagnosis to drug delivery.[1] This article emphasizes the development of naphthalene-derived, self-assemble hyperbranch polymer (PNAZO) in an aqueous medium where the azo bond works as a stimuli-responsive function in the presence of an overexpressed enzyme in hypoxic microenvironment. Here the monomer is completely water-insoluble. On the other hand, our polymer is completely soluble in an aqueous medium due to the presence of rich hydrophobicity on both sides of the monomer. Due to the amphiphilic nature of the compound and the presence of extensive hydrogen bonding, it is showing excellent twisted-rod-like morphological architecture with increasing the concentration of the polymer from below CAC to above CAC. It is well documented that the azo bond reduced very easily in the presence of azoreductage enzyme which is beautifully explained by our polymer.[2] Initially, our polymer remains nonfluorescent in the absence of azoreductage. On the other hand, in the presence of azoreductage extracted from E. coli bacterial cells, our polymer shows intense green fluorescence at 550 nm in a hypoxic microenvironment. The same phenomenon was also proved by sodium dithionite (mimic of azoreductase) for both monomer and polymer with the help of mass spectrometry and gel permeable chromatography. It is also established that our polymer can able to monitor the level of azoreductage selectively in hypoxic cell lines over normoxic cell lines.

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Optimizing Terbium-Europium Electronic Interaction by Varying Excitation Energy

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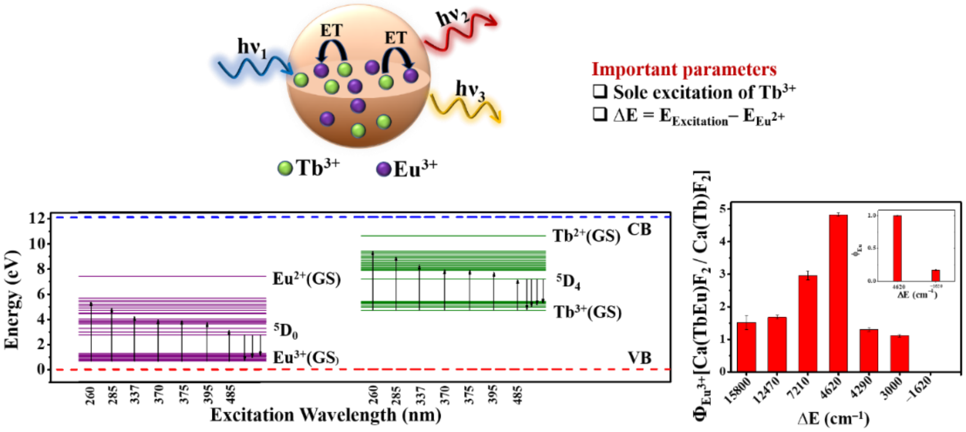
Trivalent lanthanide (Ln^{3+}) containing luminophores are gaining attraction due to their unique properties associated with longer lifetime, multiple narrow well-separated bands, and large effective shifts from excitation to emission wavelength. They can be potential candidate in the study of energy transfer. Incorporation of multiple lanthanides in inorganic nanoparticles (NPs) provides an opportunity to generate multiplex assays. This study discusses tuning the electronic energy transfer from Tb^{3+} to Eu^{3+} by varying excitation energy in CaF_2 NPs and this energy transfer process is rationalized by a charge trapping mediated process. Remarkable excitation wavelength dependent Tb^{3+} – Eu^{3+} electronic interaction is observed in the NPs and 370 nm excitation of the Tb^{3+} is found to provide optimum energy to maximize the Eu^{3+} emission. The important factors are (i) sole excitation of Tb^{3+} and (ii) maintaining the energy difference between the excitation energy and the Eu^{2+} ground energy level in the range of 4500 – 7500 cm^{-1}. This excitation energy dependence is found to be inefficient in the bulk medium. Finally, these experimental outcomes clearly provide a picture under which optimum Tb^{3+} – Eu^{3+} electronic interaction can be obtained from inorganic NPs for suitable photoluminescence applications.



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Singlet Fission in Anthracene Solution: Role of Correlated Triplet-Pair

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Singlet fission (SF), a process generating multiple excitons, efficiently harnesses excess energy from high-energy photons in photovoltaics, has potential to overcome the limit on power conversion efficiency of 33%, the Shockley-Queisser limit.[1,2] SF was first observed in anthracene crystals,[3] however, it is never reported in its solution. SF is reportedly mediated by elusive correlated triplet-pair state, ^{1}(TT) state.[4] This work presents direct spectroscopic evidence of ^{1}(TT) state following SF in anthracene in toluene. Using time-resolved fluorescence spectroscopy, we have observed temperature-independent formation of ^{1}(TT) state as a SF intermediate; an iso-emissive point in time-resolved area-normalized emission spectra reveals a single-step population transfer from S_1 to ^{1}(TT), resulting from SF (Figure a, b).[5] Interestingly, fate of ^{1}(TT) is temperature-dependent: it forms free triplets at 298K, excimer-like species at 77K. At low-temperature, 0-0 vibronic peak of emission spectra of thin film is observed to show pronounced emission. Superradiance is reported to be efficient at low-temperature due to delocalisation of triplets.[6] This confirms that free triplets are being formed. Energetics were calculated theoretically (T_1) and experimentally (S_1 and ^{1}(TT)) and show that SF occurs endothermically in anthracene solution, with requisite energy being facilitated by interplay between formation of ^{1}(TT) state and anthracene's C-H stretching vibrational modes.

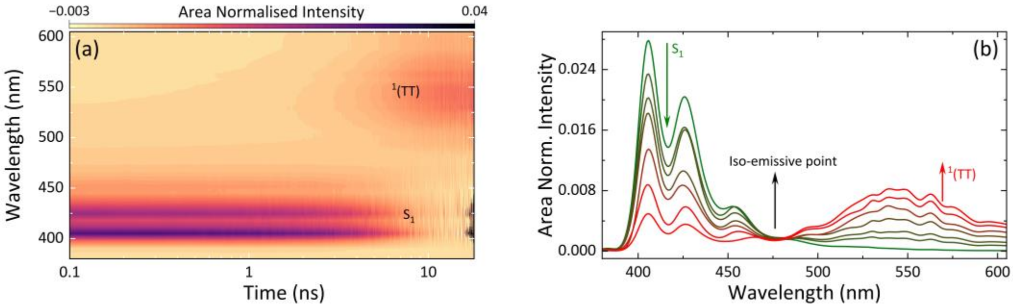

Figure 1. Graphical abstract.

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Stable Diradical on the Dimethyldihydropyrene Scaffold

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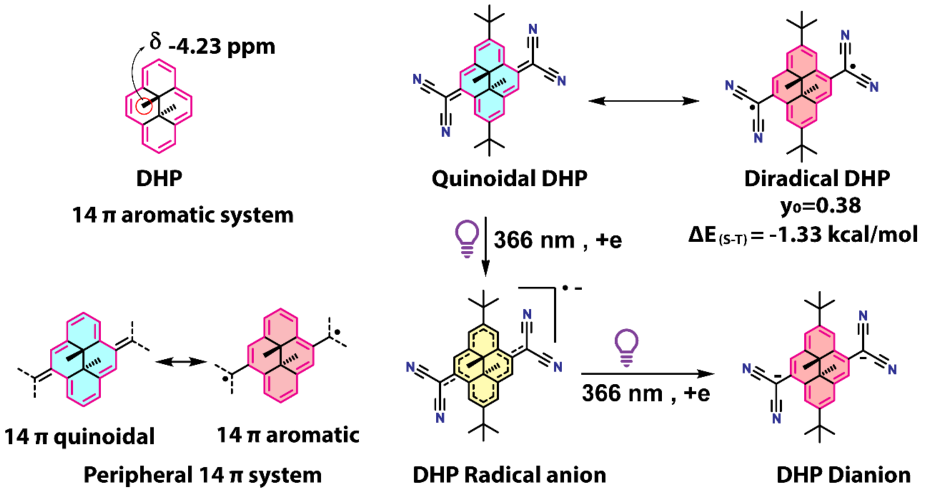
Quantum information processing has seen significant progress in recent times, with the introduction of various qubit platforms based on systems such as nuclear spins, trapped ions, and photons. More recently, the use of electron spin to construct qubits has been explored. Organic diradicals or radicaloids have also been considered as potential qubit systems. However, these species are typically short-lived and highly reactive due to the presence of two unpaired electrons in singly occupied molecular orbitals, which poses a significant challenge to their study and practical applications under standard laboratory conditions. To address this challenge, we chose to explore Boekelheide's dimethyldihydropyrene (DHP), a 14 π aromatic framework, and perturbed its aromaticity by constructing its "masked aromatic" quinoidal form. The perturbed aromaticity of this system was apparent through various methods such as X-ray diffraction, and NMR chemical shifts which was supportd by quantum chemical calculations. Upon formation of the biradical structure, centered on the two exocyclic carbons, the molecule restored its aromaticity. In addition, the diradical could be converted to a radical anion upon photoexcitation, and a dianion species through consecutive excited-state electron transfer when dimethylformamide was used as a solvent.



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Assembly-Induced Emission in Silver Nanoclusters and Mechanistic Elucidation of their Catalytic Activity

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The phenomenon of Aggregation Induced Emission (AIE) is an emerging strategy to tune the optical properties of luminescent Metal Nanoclusters (MNCs). Our present investigations delineate the remarkable tuning of the photophysical properties of weakly luminescent mercaptosuccinic acid (MSA) templated silver nanoclusters (AgNCs). Upon AIE of AgNCs through the introduction of Zn^{2+} ions, the emission maximum of AgNCs was shifted from ~465 nm to ~670 nm with an unusual augmentation in photoluminescence intensities (~3000 times). The minimization of energy dissipation due to the formation of Zn^{2+} induced rigid assembly mainly accounts for these unprecedented optical signatures. Consequently, the otherwise weakly emissive AgNCs system (Quantum Yield, QY ~0.1%) gets converted to a highly luminescent red-emitting Zn^{2+} induced AgNCs assembly (Zn-AgNCs, QY ~2%).[1] Such metal ions-induced surface modification of AgNCs opens the possibility of exploring the role of the core and ligand shell of AgNCs in their catalytic activity. A facile surface modification of mercaptosuccinic acid (MSA)-templated AgNCs has been selectively achieved through Mg^{2+} ions (Mg-AgNCs). Our spectroscopic and microscopic experiments revealed that the negatively charged AgNCs efficiently catalyze the reduction of 4-nitrophenol (4-NP) with a rate constant of 0.23 ± 0.01 min^{-1}. However, upon surface modification, the catalytic efficiency almost doubles due to the formation of Mg-AgNCs. The catalysis through AgNCs and Mg-AgNCs collectively portrays the role of the metallic core and electrostatic surfaces.[2]

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Pathways to Mn Emission in a Mn-Doped 2D Hybrid Halide Perovskite

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We have investigated the mechanism of Mn emission in Mn-doped BA_2PbBr_4 single crystals with the help of temperature-dependent Mn emission studies. Our results reveal that the host-to-dopant energy transfer is the primary mechanism of sensitizing the Mn states; this is achieved by energy transfer from the lowest-energy host excitonic state to the energetically nearest Mn^{2+} multiplet state. These excited Mn multiplet states subsequently relax to the first excited multiplet, $^4T_{1g}$ state via Mn d-d deexcitations. Since the relevant multiplets[1] have larger energy differences than the highest energy LO phonon at 59 meV [2],[3] in BA_2PbBr_4, this relaxation requires multi-phonon processes, experiencing a phonon-bottleneck at lower temperatures, and therefore, suppressing the Mn emission intensity at lower temperatures. In contrast to the $CsPbCl_3$ nanocrystal host, the Mn emission intensity is not strongly suppressed at low temperatures in this 2D layered perovskites due to the presence of higher energy phonon modes (59 meV) compared to the $CsPbCl_3$ nanocrystals (28 meV); this helps to enhance the multi-phonon emission rate, and therefore, decrease the temperature dependence of the Mn emission intensity.

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Ultrasensitive Piezochromic Molecular Crystals: Pressure-Induced Controlled Regulation of Thermally Activated Delayed Fluorescence and Long Persistent Luminescence

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The basic rule of nature states that the total entropy of an isolated system rises continuously without an external force until and unless the system attains disorganisation and chaos. Hence, application of an external agent to regulate and control the attainment of chaos is necessary for its fruitful application. Thinking in the same direction, regulation of thermally activated delayed fluorescence (TADF) and room temperature phosphorescence (RTP) was necessary for a fluorophore to survive and show its characteristic nature. Here, it has been demonstrated successfully that a carefully designed novel pyrene derivative exhibits remarkable aggregation-induced emission (AIE) overcoming the characteristic fast excitonic decay of pyrene compounds. It has been established that J-aggregation in the red-emitting molecular crystals of the compound reduces the singlet-triplet gap (ΔE_{ST}), allowing TADF with a very high photoluminescence quantum yield (PLQY) of 72%. Anisotropic grinding of the crystals leads to the generation of well-defined microcrystals that show RTP as the aggregating nature changes. Impressively, under isotropic hydrostatic pressure, the crystals show near-infra-red (NIR) emission with a very high piezochromic luminescence sensitivity of 46.2 nm/GPa. It is established that formation of stabilised H-aggregation in the self-assembled microcrystals is responsible to generate the ultra-long RTP. A highly sophisticated full spectrum Mueller-matrix analysis is used for the first time in such systems to demonstrate the details of the effect of perturbation (pressure) on the molecular conformations.

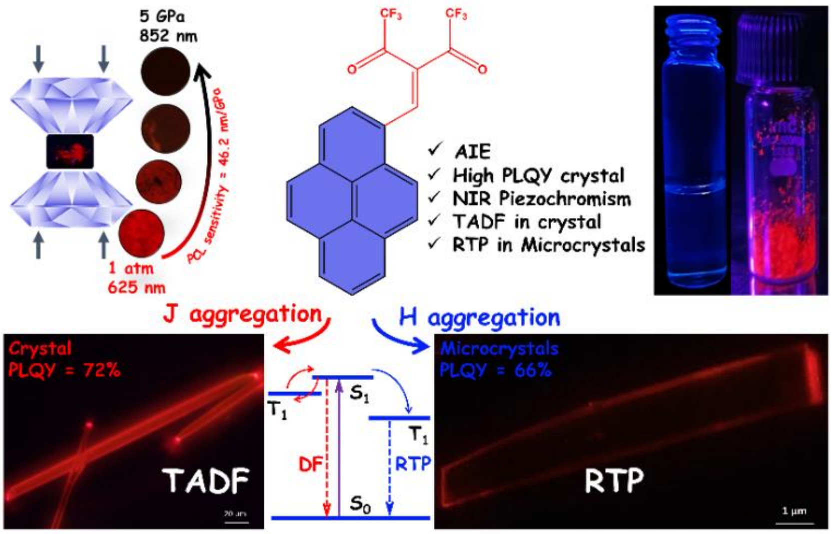

Figure 1. Graphical abstract.

Exciton Dynamics in Freely Diffusing Doped CdSe Nanotetrapods

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Doping with Ag^+ and Cu^+ brings about an enhancement in the photoluminescence (PL) of oleic acid capped CdSe nanotetrapods (NTPs) in toluene.[1] This phenomenon is attributed to the longer times required for radiative excitonic recombination between delocalized electrons in conduction band and localized holes in dopant states. The microsecond blinking dynamics of these NTPS has been investigated using fluorescence correlation spectroscopy (FCS). With increasing power, the initial correlation function G(0) decreases significantly for doped and undoped NTPs due to photoactivation. However, the extent of decrease is higher for doped NTPs than for the undoped one. Photoactivation, photoinduced transformation of dim/dark to bright particles within the confocal volume, are observed at higher excitation power.[2] Excitonic recombination pathways become more homogeneous upon doping. With increasing power, blinking time decreases significantly for both the cases. However, the extent of decrease is lesser for doped one. The faster on-off time is triggered by Auger recombination which is suppressed significantly upon metal doping due to breakdown of electron-hole correlation.[3] Both blinking and photoactivation are intimately linked to charge separation efficiency and dynamics of nanocrystals and are necessary criteria for their application in photovoltaic and optoelectronic devices.

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Lysosome-Targeting Hydroxyquinoline-Derived Small Molecule Turn-On Fluorescent Probe for Alzheimer's Disease Detection and Diagnosis

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In the pursuit of effective Alzheimer's disease (AD) diagnostic tools, we offer a novel small-molecule fluorescence probe designed to specifically target lysosomes, important organelles implicated in AD pathology. When interacting with amyloid beta, this hydroxyquinoline-derived probe exhibits a distinctive turn-on fluorescence response, allowing for sensitive and precise detection of AD. The probe's design takes use of the specific lysosomal abnormalities seen in Alzheimer's disease, providing a viable technique for early-stage diagnosis. The molecular tool given here has enormous potential for furthering our understanding of AD pathophysiology and allowing the development of novel diagnostic techniques for improved patient outcomes.

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Unravelling the Photo-Physics of $CsPbBr_3$ Nanocrystals for Optoelectronic Device Applications

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Lead halide perovskite nanocrystals (PNCs) have emerged as highly promising alternatives to traditional semiconductor nanomaterials for photovoltaic applications. Focusing on the importance of interfacial charge transfer (CT) between different layers of solar cell in improving its performance, we have elucidated the CT process between $CsPbBr_3$ PNCs and Fullerene (C_{60}) molecules using various steady-state and time-resolved spectroscopic measurements. We observed a facile electron transfer (ET) from $CsPbBr_3$ PNCs (donor) to C_{60} (acceptor) as is evident from their energy level alignment indicating a plausible efficient ET. Further, we have studied the electron transport properties using current sensing atomic force microscopy (CSAFM) across the electrode-PNC-electrode nanojunction and observed a significant increase in conductivity with the insertion of C_{60} molecules. To unveil the significance of ET in such devices, we simulated the performance of two different device structures: FTO/$CsPbBr_3$/PEDOT:PSS/Au and FTO/C_{60}/$CsPbBr_3$/PEDOT:PSS/Au with C_{60}. FTO serves as the transparent electrode, $CsPbBr_3$ as the photo-active layer, PEDOT:PSS and C_{60} as the hole/electron transport layer. Our findings revealed that inclusion of the band-aligned C_{60} layer to PNCs increased the power conversion efficiency from 16.94% to 20.49%. This study highlights the importance of modulation in interlayer charge transfer in regulating the efficacies of photovoltaic devices.

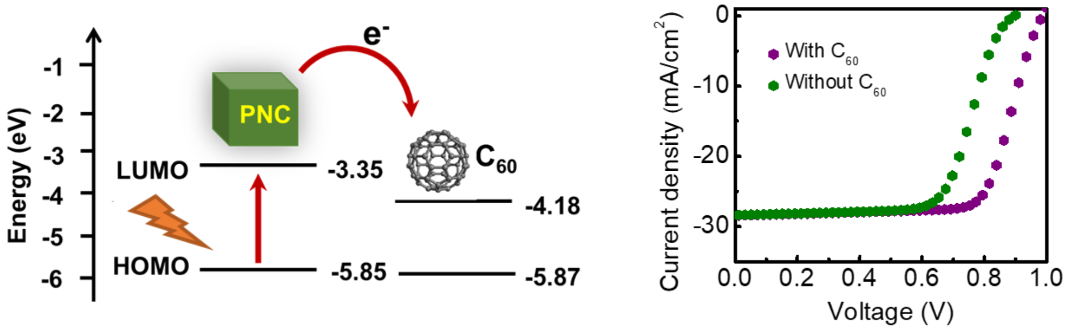

Figure 1. Energy band alignment representing ET between $CsPbBr_3$ PNCs and C_{60} molecules, and Simulated J-V curve of two devices, without and with C_{60} as ETL.

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Synthesis, Characterization and Application of Carbon Quantum Dots (CQDs) for Imaging Giant Unilamellar Vesicles (GUVs) using Fluorescence Microscopy

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Carbon Quantum Dots (CQDs) are at the core of luminescence and fluorescence imaging as emerging and promising labeling choice owning to their higher molar absorption coefficient, photochemical stability, lifetimes, surface tunability and lower photobleaching in comparison to those of organic dyes. Interestingly, their lower toxicity and higher solubility in water compared to inorganic QDs such as CdTe, CdSe QDs make them more suitable fluorescent agents for biological applications.[1] Giant Unilamellar Vesicles (GUVs) are one of the most useful model systems to study the membrane related processes in a controlled manner.[2] They are an important tool for researchers in studying interactions between lipids and proteins. The study of interactions involving uptake and permeability of different sizes, charges of CQDs through membranes of GUVs can provide insights into understanding the coulombic interactions occurring between CQDs and GUVs membranes.[3] In regard to cellular environment, these studies can open new perspectives. In this poster presentation, I will discuss the synthesis, detailed characterization and the application of purified CQDs fractions in bioimaging of GUVs using fluorescence microscopy technique.

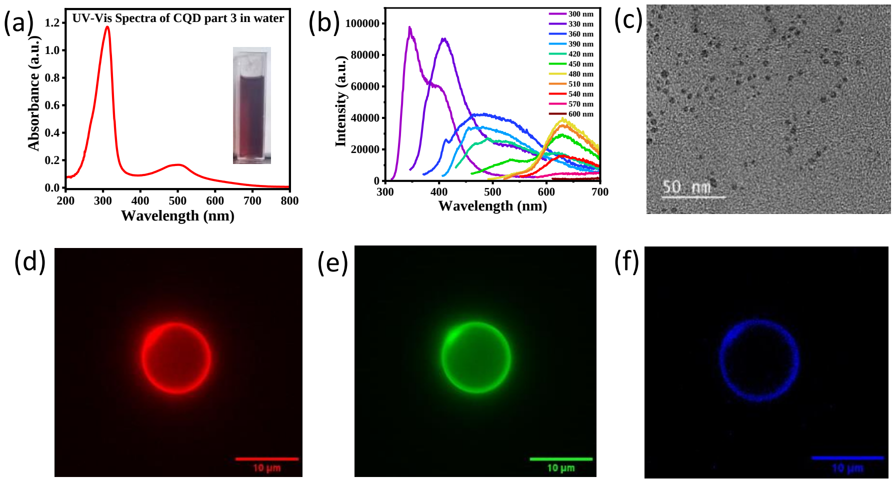

Figure 1. (a) UV-Vis spectra, (b) photoluminescence spectra, (c) TEM image of CQDs, and (d), (e) &(f) GUVs imaging with CQDs using fluorescence microscopy technique in TRITC, FITC & DAPI filter, respectively.

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Deciphering the Proficiency of Aliphatic/Aromatic Functionality on Heteroatom Embedded Planar Polycyclic Core: Towards an Advanced Onsite Detection of Tetracycline and Oxytetracycline

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The development of planar luminogens with isoelectronic B-N moiety and replacing the conventional C=C bonds is an unusual approach to tune the optical properties of organic materials in solution and condensed phase. Herein, three boron congeners and their analogous carbon congeners are developed via engineering the aliphatic / aromatic functionality unveiling the role of each functionality on intermolecular packing and luminogenic behavior.[1] The boron-fused molecules exhibited slip-stack packing orientation governed by B-π interactions and showed aggregation induced emission in the condensed state unlike the carbon analogs which had a typical aggregation caused quenching (ACQ) phenomena. Notably, the offset dimeric arrangement in octyl chain substituted boron congener offers highly emissive nano-assemblies and solid-state luminescence which was utilized for fluorescence-based rapid detection of broadly used tetracycline and oxytetracycline antibiotics. This detection was further translated into a prototype technique using a smartphone-based platform for easy, onsite detection. Examining the structure-property relationship could lead to the development of highly emissive unusual luminogens by restricting the detrimental π-π stacking via insertion of BN moiety into cyclic hydrocarbon framework. This promising strategy provides access to potential planar luminogens while generating unusual photophysical properties for advanced applications.

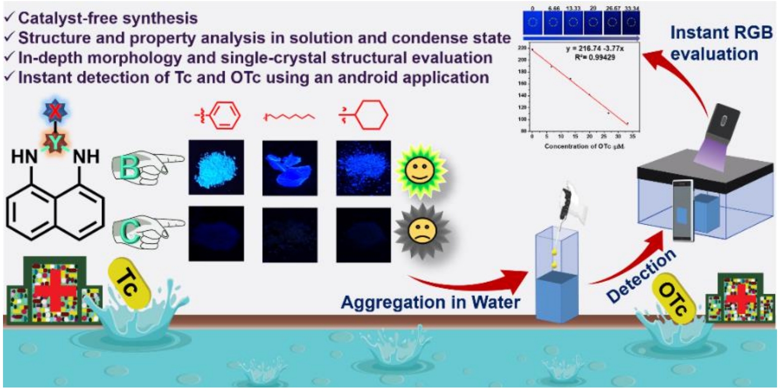

Figure 1. Graphical abstract.

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Effect of Dopants on the Nonlinear Optical Properties of 2D Layered Organic-Inorganic Lead Halide Perovskites

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Hybrid lead halide perovskite compounds have emerged as one of the leading candidates for optoelectronic applications and have accomplished the most notable progress in the field of nonlinear optical properties due to strong quantum and dielectric confinement. Recent interest in developing doped layered 2D lead halide perovskite due to their improved stability, rich structural flexibility, and magneto-electric properties, make perovskites much more functional than their undoped counterparts. [1,2] Despite the wide ongoing research in achieving record efficiencies in solar cells and other photonic/optoelectronic devices using lead halide perovskites, there are very less reports regarding the nonlinear optical properties of the doped halide perovskites.[3] Nonlinear optics are extremely important for photon energy conversion, light manipulation, and other optical technologies.[4] Therefore, we have explored the third-order nonlinear optical (NLO) response in the form of third harmonic generation (THG) of the Mn^{2+} or Sb^{3+} doped phenethylamine lead iodide (PEA_2PbI_4) for the very first time. Nonlinear optical effects are expected to be stronger due to the presence of the defect states acting as optical transition channels. The comparison further revealed the high NLO properties and optical stability of the doped crystal system, making it suitable for real application purposes.

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FRET-Driven Temperature Sensing using Pyrene-C102 Loaded Hybrid Niosome with High Relative Sensitivity and Reversibility

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Optical thermometers based on fluorescence intensity are crucial for their high sensitivity, non-contact temperature sensing, and exceptional repeatability. In this study, we present fluorescence resonance energy transfer (FRET)-based ratiometric temperature sensing employing pyrene (donor) and coumarin 102 (acceptor) loaded in hybrid niosomes composed of span 60 and pluronic L-64. Under 335 nm excitation, as the temperature increases from 20 °C to 50 °C, the fluorescence emission intensity of pyrene decreases, while that of coumarin 102 (C102) increases. This leads to a ratiometric detection of temperature within the biological range. This highly reversible phenomenon is attributed to the phase transition of the hybrid niosomes. The fluorescence intensity ratio (FIR), defined as the emission intensity of pyrene at 394 nm to the emission intensity of C102 at 469 nm, is employed to calculate the relative sensitivity of the sensor. The remarkable relative sensitivity of the sensor is determined to be 9.4%°C^{-1}, with a temperature resolution of 0.00156°C^{-1} at 42°C, which stands among the best values reported till date.[1] These findings indicate that the designed pyrene-C102-loaded hybrid niosomes are a promising candidate for application in optical temperature sensing for the detection of diseases within the biological range.

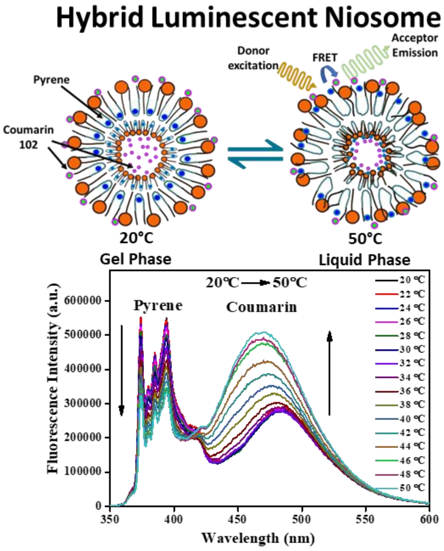

Figure 1. Graphical abstract.

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Information-Theoretic Measures and Compton Profile of H Atom under Finite Oscillator Potential

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Information-theoretic measures for *nl* (^{2}L) states of H atom (with n = 1-10 and l = 0-2, where n and l denote the principal quantum number and angular momentum quantum number, respectively) have been investigated within a quantum dot (QD) by utilizing the Ritz variational principle with the help of a Slater-type basis set. A well-established two-parameter (depth and width) model finite oscillator (FO) potential is used to characterize the dot environment.[1] The variationally optimized position space wavefunction is utilized to determine the momentum space wavefunction, leading to the generation of the momentum space radial density distribution. We have explored the impact of cavity parameters on quantum information theoretic measures, such as Shannon and Fisher information entropy, for H atom in the ground as well as in various excited states within QD.[2,3] New scaling laws pertaining to Shannon and Fisher entropy have been proposed. The momentum space radial density is employed to derive the Compton profile of the confined H atom.[4] Possible tunability of Shannon entropy, Fisher entropy and Compton profiles *w.r.t.* the quantum dot parameters are noted.

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Are the Same Design Rules for Engineering Ferroelectricity in Inorganic Perovskites Valid in their Hybrid Counterparts?

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Considering the well studied titanate family of the inorganic perovskites AtiO3, where A is an alkali metal atom, one finds that a large ion at the A site is able to induce an off-centering of the Ti atom, and thereby stabilize a ferroelectric ground state. The size of the A site cation plays a role in increasing the volume of the unit cell, and thereby decreasing the hopping as well as the Coulomb interactions related cost involved in the off-centering. The question we ask here is whether a similar mechanism is at work in hybrid perovskites, that allows ferroelectricity to be stabilized.

Recently, a class of phosphonium based molecules have been used at the A site of Pb-Br based perovskites, and the large tolerance factor leads to one-dimensional perovskites being stabilized.[1] Solving for their structure[1] within ab-initio density functional theory based calculations, we find that ferroelectric distortions are stabilized in the inorganic network, while each of the molecules has no net dipole moment. We will present our analysis to understand the mechanism involved as well as its extension to other molecules at the A site.

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Temperature-Assisted Molecular Reordering in *n*-type Organic Semiconductor Films: Impact on the Nanoscale Morphology, Photophysical Properties and the Charge Carrier Transport

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Charge carrier transport in bulk organic semiconductors, especially in solution-grown films, is invariably dictated by the semiconductor nanoscopic morphology and molecular level organization of the charge hoping centers. Tiny positional displacements of such units can lead to a significant alteration of the bulk carrier transport. Various pre- and post-film deposition techniques have been widely used to achieve suitable layer morphology and molecular arrangement on the desired substrates. Herein, we demonstrate our findings on temperature-assisted morphological restructuring inducted by molecular scale reordering of *n*-type molecular semiconductors on device substrates. A series of positional isomers of end-substituted napthalenediimide (NDI) derivatives were subjected to study. Mainly for one derivative, *m*-Picolylnaphthelenediimide (*m*-PyNDI), a dramatic improvement in field-effect electron mobility and the device performance was evident upon such post-deposition treatment. Subsequently, a series of investigations starting from the bottom level *i.e*, molecular scale aggregates in solution state which is expected to follow a thermodynamically driven assembly pathway to the bulk films, were carried out systematically and are summarized here. Spectroscopic signatures of the aggregates were carefully studied by following the exciton coupling model, and the evolution of morphological transformation was monitored using microscopic techniques. A correlation between the solution state and the substrate-assisted assembly, the effect of thermal annealing and, thereby, improvement in the device performance is explained here.

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Ultrafast Electron Transfer and Prolonged Exciton Recombination are Achieved by Squaraine Encapsulation in the Carbon Nanotube

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Carbon nanotubes (CNTs) are one of the emerging 1D materials, has significant contributions towards solar and optoelectronic applications. To construct highly efficient photovoltaic, electron transfer (ET) should be fast; meanwhile charge recombination must be suppressed. The hollow cores of larger diameter CNTs can allow encapsulation of various molecules. Applying self-consistent-charge density-functional tight-binding (SCC-DFTB) theory combined with nonadiabatic molecular dynamics (NAMD),[1] we demonstrated that interfacial ET from outer and encapsulated 3 squaraine (SQ) to 9-8 CNTs occurs within 152 and 154 fs respectively. The simulated ET time scales for encapsulated 3SQ@CNT are nicely corroborated with the experiment (200 fs).[2] When 6SQ molecules are encapsulated in the CNTs (6SQ@CNT), the ET is quickest (45 fs). Smaller band offset and larger NA coupling accelerates ET. Conversely, the nonradiative e-h recombination takes place on 173 ps and 1.93 ns in outer and inner 3SQ@CNT composite respectively. However, the prolonged exciton life time exhibits by 6SQ@CNT hybrid with a time constant of 5.02 ns. This phenomenon is explained by larger band gap and smaller NA coupling at the band edge. Our investigation unravelled the effect of encapsulated SQ on the fundamental charge transfer dynamics and provided valuable information for future photovoltaic utilization.

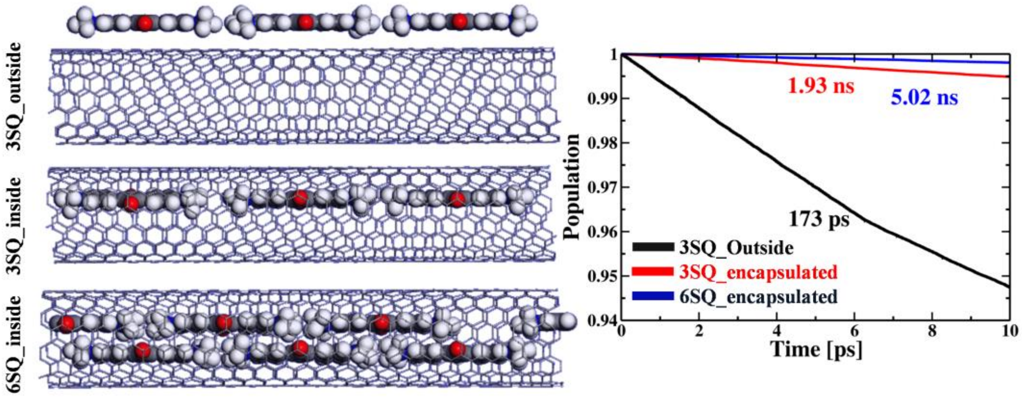

Figure 1. Optimized geometries and first excited population decay of various CNT@SQ nanohybrids.

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Fabrication of Cobalt Oxalate Supported Non-precious Electrocatalyst for Improving Alkaline Water Oxidation Activity

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Carbon-free sustainable energy sources have been engrossed immensely in recent times. The utility of hydrogen as a fuel is one of the most convenient and eco-compatible approaches due to its high specific energy density (142 MJ/kg) and zero-carbon emission. On the way of increasing hydrogen production, electrolysis of water can be tricky because of sluggish oxygen evolution reaction (OER) kinetics. To trigger the electrochemical process, a non-precious electrocatalyst is urgently required with abundant active sites, long-term alkaline stability and simple preparative protocols for bulk-scale yield. Cobalt oxalate was primarily prepared as a synthetic precursor using oxalic acid-based ligand-assisted wet-chemical synthesis. To enhance the OER performance, a cobalt-iron oxalate-based pre-catalytic framework was strategically developed showing just 295 mV overpotential to reach the benchmark current density of 10 mA/cm2. In addition, hydrogen evolution reaction (HER) was also checked by cobalt oxalate assisted cobalt selenide framework that further requires 140 mV overpotential to reach -10 mA/cm2 in 1M KOH. An alkaline electrolyzer was finally constructed employing cobalt-iron oxalate as anode and cobalt selenide as a cathode for impressive electrochemical water splitting performance in alkaline conditions. The overall synthetic strategy unlocks the simple preparative method without using any precious elements for real-world implementation.

Keywords: Cobalt-Iron Oxalate, Cobalt Selenide, Oxygen evolution reaction, Hydrogen evolution reaction, Alkaline Water Splitting.

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Super-Bright Zn-Alloyed $CsPbI_3$ Perovskite Nanocrystal: Ultrafast Dynamics and Single Particle Spectroscopy

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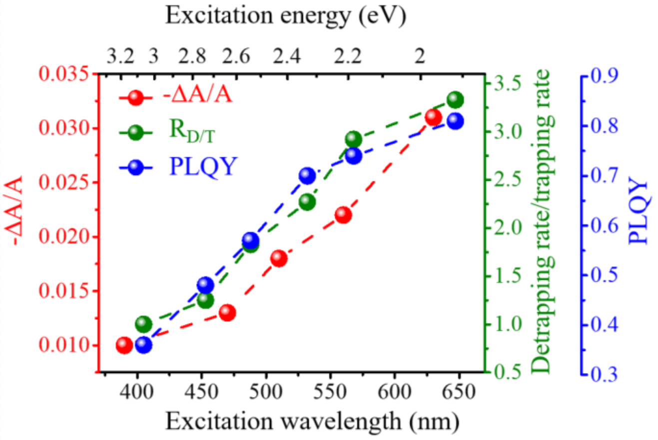
Perovskite nanocrystals (PNCs), specifically $CsPbI_3$ PNC, due to its unique optical properties are in great demand for various applications.[1] Employing ultrafast dynamics and single particle spectroscopy[2,3] in super-bright (~$1x10^8$ $M^{-1}cm^{-1}$) Zn-alloyed stearic acid coordinated $CsPbI_3$ PNC, upon increasing λ_{ex}, following interesting observations have been made: (i) hot-carrier-cooling-time decreased (756-107 fs), (ii) amplitude of charge-carrier-trapping decreased (0.74 to 0.41), whereas, (iii) amplitude of radiative recombination increased (0.26 to 0.59) and (iv) normalized-bleach-amplitude (-ΔA/A) increased (0.010 to 0.031), (v) peak of ON-fraction increased (64 to 90%), (vi) ON-truncation-time increased (3.6 to 8.3 s), and (vii) detrapping rate/trapping rate increased (1.0 to 3.3). Change in the magnitude of all these parameters could be correlated with λ_{ex} dependent PLQY (Fig. 1).



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Visible-Light Triggered Water-Soluble Polymeric Peroxynitrite Generator in Cancer Therapy

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Nitric oxide (NO) serves as an intrinsic signalling molecule with diverse therapeutic applications.[1,2] However, it exhibits concentration-dependent physiological effects. Typically, lower concentrations (pM – nM) of NO contribute to vasodilation, cardiac relaxation, angiogenesis, and similar functions, while higher concentrations (> 1 μM) can be employed for anticancer and antibacterial activities. In this study, we have developed a water-soluble *N*-nitrosamine[3] based polymeric material (**BCPx-NO**) with anthraquinone, which is capable of releasing NO, reactive nitrogen species (RNS), and reactive oxygen species (ROS) under visible light irradiation. **BCPx-NO** releases NO in the range of 40-65 μM within 10 h of photoirradiation. Additionally, it generates singlet oxygen species ($^1O_2$) and peroxynitrite ($ONOO^-$) under blue light irradiation (427 nm, 2.25 mW/cm^2). To comprehend the NO release mechanism, a small molecular NO donor (**NOD**) was synthesized, sharing chemical resemblance with the functional unit of **BCPx-NO**. Further investigations reveal that **BCPx-NO** and **NOD** undergo photolytic cleavage after NO release under photoirradiation, forming anthraquinone and the corresponding aldehyde. This spatiotemporally controlled $ONOO^-$ and $^1O_2$ generator exhibits toxicity against human breast cancer cells, MDA-MB-231, and intracellular ROS/RNS generation is confirmed through various fluorescent probes using fluorescence-activated cell sorting (FACS) and confocal imaging studies.

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Tuning Crystal Plane Orientation and Sculpturing the Facets in $CsPbBr_3$ Perovskite Platelet Nanocrystals

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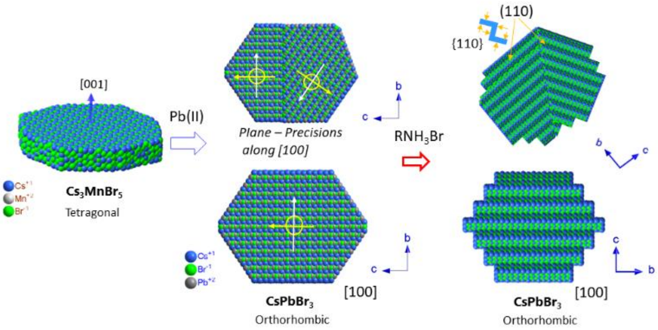
Two-dimensional-shaped $CsPbBr_3$ platelet nanocrystals are widely studied for their bright high energy emission and self-assembly. These nanostructures are in orthorhombic phase, have a square shape, and have the vertical axis [001] perpendicular to the basal plane. Moreover, these are mostly single-crystalline structures with a continuous lattice and appear like slices of cube nanocrystals. In contrast, herein, multijunction and hexagonal single crystalline nanoplatelets of $CsPbBr_3$ are reported to have all their vertical axes [100]. These are obtained by using the perovskite derivative of tetragonal Cs_3MnBr_5 as the parent material and subsequent B-site Pb(II) introduction in the presence of phenacyl bromide at different reaction temperatures. When oleylammonium bromide was added to these postsynthesized platelets, all six edges and two planar facets are transformed from flat to wavy structures. With a variation in concentration, the crest-to-crest distance of these wavy platelets are also tuned. These became possible because of the oleylammonium ions, which changed the {200}, {012} and {020} facets of orthorhombic phase of $CsPbBr_3$ to the more compatible {110} and {002} facets simply by surface atom dissolution. While shape modulations in ionic halide perovskite nanocrystals still face synthetic challenges, these results provide strong evidence for shape variation in these nanostructures.



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Observation of Hot-Phonon Bottleneck Effect in Perovskite Quantum Dots: A Femtosecond Optical Gating Study

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Thermalization, the major loss channel, limits power conversion efficiency in photovoltaics to ~33%, the Shockley–Queisser limit.[1] Above bandgap excitation generates hot-carriers (HC) which thermalize and cool down to the band edge, dissipating excess energy as heat to the lattice.[2] Understanding HC is crucial, as efficient extraction of HC has potential to increase efficiency of photovoltaics. Hot-phonon bottleneck (HPB) effect, a fundamental way of tuning carrier cooling, is observed at comparatively high carrier densities when emitted optical phonons are reabsorbed by carriers. We are applying time-resolved emission spectroscopy to observe HC dynamics in perovskite quantum dots, ($CsPb(Cl/Br)_3$). Time-resolved emission spectra (TRES) show a shift in peak position as well as change in spectral shape. Origin of this shift can be HC cooling.[3] However, any additional dynamic process can also lead to shift in peak frequency, leading to inaccurate results. We have analysed the TRES using a full line shape model, which is convolution of Gaussian with Maxwell-Boltzmann distribution,[4] (figure 1b). This analysis focuses on hot carrier cooling reflected in high energy tail of TRES irrespective of any other processes present. HPB effect slows down carrier cooling due to reabsorption of optical phonons, (figure 1c). Additionally, higher excess energy leads to higher carrier temperatures.

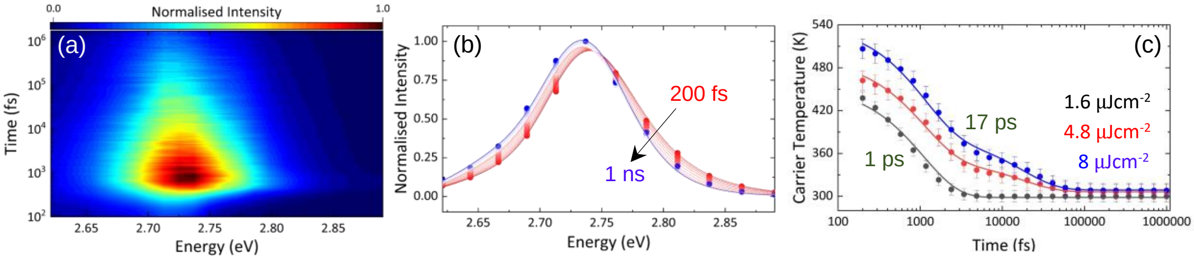

Figure 1. (a) False color map of TRES. (b) Full line shape fitting of normalized TRES at different times (c) Carrier cooling curves (dotted) at different excitation densities (fitting - solid lines) showing hot phonon bottleneck effect.

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Nanoparticle Organic Network Mediated Enhanced Optoelectronic Properties of Semiconducting Polymer Field Effect Transistors

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Semiconducting conjugated polymers exhibit morphology consisting of crystalline and amorphous regions in thin films. The orientation of the crystallites (edge-on versus face-on), a fraction of the crystalline region, and the interconnection between the aggregates play significant roles in tuning the optoelectronic properties and charge transport of conjugated polymers. We introduced nanoparticle organic networks (NONs), which are covalently connected metal nanoparticle nodes with organic linkers, in the semiconducting polymer-based field effect transistors. Upon introduction of the NONs, we observe that the field effect mobility (μ_{FET}) increases by two orders of magnitude and photoresponsivity of the semiconducting polymer is enhanced by 760%. This improvement was attributed to the structural ordering induced by NONs within the semiconducting polymer, along with the effective passivation of trap states as well as enhancement in the conjugation length.

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Spectroscopy and Dynamics of Beta-Lactoglobulin Complexed with Rifampicin

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Beta-Lactoglobulin(BLG) is an important whey protein that has wide range of medicinal and drug delivery applications mainly due to its stable nature in even the acidic environment of stomach.[1,2] Tuberculosis is well-known for its severity among the disease community and drug delivery approach is also one of the potential approaches to tackle against it. In this study, a widely used anti-TB drug named Rifampicin(RIF) was investigated with BLG protein. To estimate the potential of BLG protein as RIF carrier, we used several biophysical tools. Fluorescence of tryptophan(Trp) amino acid in BLG was monitored to characterise and analyse the binding interactions with RIF. The nature of quenching was determined from time-resolved fluorescence spectroscopy and temperature-dependent studies. From thermodynamic characterisation, we found that hydrophobic interactions are involved that were supported by extrinsic probe study via 8-anilino-1-naphthalene sulfonate(ANS) fluorophore. From FTIR spectroscopy we measured the secondary structural changes in the protein and found that beta-sheet content was increased on the cost of helical content supported from Molecular Dynamics(MD) Simulation studies. Further, we measured Förster resonance energy transfer(FRET) mechanism involved from BLG Trp to RIF. This study will extend the potential of BLG protein and will help to understand drug-protein interactions.

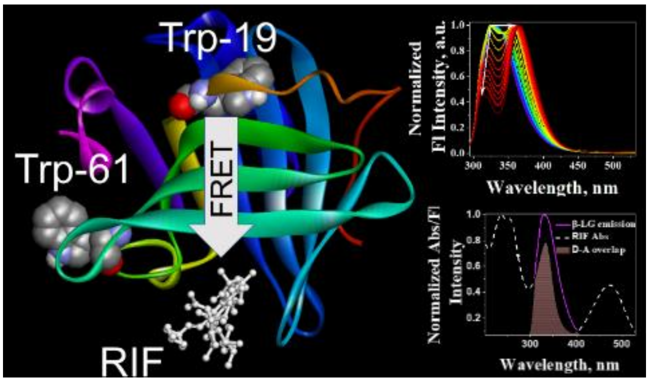

Figure 1. Characteristic binding analysis of rifampicin with beta-lactoglobulin by spectroscopy, molecular docking and molecular dynamics simulation.

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Molecular Self-Assembled Structures of Small-Peptide Glutathione on the Surface of Gold and Silver Nanoparticles for Targeted Drug Delivery

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Recently nanoparticles oriented research is an area of interest due to its various potential applications in medical, chemical, and biological fields. Functionalized nano-materials gain a lot of significance because of their many attractive properties such as biocompatibility, ligand functionalization, plasmonic activity. Over the past few years metal nanoparticles play a key role in modern medicine being a carrier for drug delivery to the target cells. Constancy under appropriate physicochemical environments has a challenging requirement for such in vivo applications. Gold and silver nanoparticles have higher surface energy, for which these spherical nanoparticles incline to aggregate in ionic solutions that can limit their applications. For overcoming such limitations, various coating agents like organic molecules, peptides proteins, etc. are extensively used which can reduce the surface energy to increase solubility in ionic solution. Among these capping agents, peptides provide invaluable support in material sciences by interacting with the surface of noble metal nanoparticles. The structural conformation of a self-assembled monolayer of these capping layers have a massive effect on various nanoparticles such as it can assist for proficient cell membrane penetration and targeted drug delivery. These studies mainly focused on structural determination of peptide coating layers on gold and silver nanoparticles.

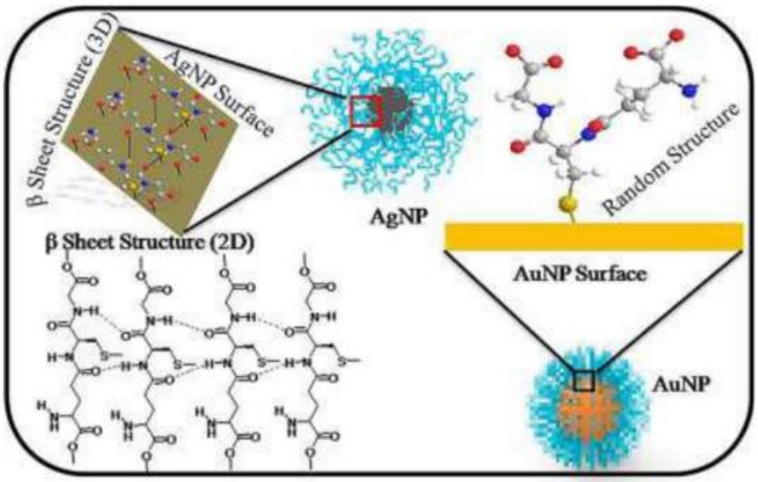

Figure 1. Model surface structure of Glutathione on Silver [AgNP (left)] and gold [AuNP (right)] nanoparticles.

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Beneficial Intrinsic Hole Trapping and its Amplitude Variation in an Ultra-Stable, Highly-Bright, Toxic-Metal-Free Quantum Dot

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Unlike electron trapping/detrapping dynamics, both intrinsic (i.e. without using any external agent) hole-trapping and detrapping phenomenon have not been observed in any quantum dot (QD) or perovskite nanocrystal (PNC).[1] For toxic-metal-free, small-sized (~3.3 nm), highly photo-luminescent (PLQY = 96%) (Fig. 1a) and extremely stable (Fig. 1b) $CuInS_2/ZnSeS$ Core/Alloy-Shell (CAS) QD,[2] such observation has been for the first time.[3] Moreover, no variation in amplitude of intrinsic hole-trapping (or detrapping) has been reported for any QD/PNC. For $CuInS_2/ZnSeS$ CAS QD, very significant amplitude variation of intrinsic hole-trapping (~16 to ~42 %) and intrinsic hole-detrapping (~44 to 23%) have been observed, for the first time in the entire QD family/PNCs.[3] Unlike, detrimental electron-trapping,[4] intrinsic hole-trapping has been noted to be quite beneficial towards increasing PLQY value up to 96%.[3] Simultaneous trapping of both electron and hole lead to the longest ON duration (>2 minutes) reported for any toxic-metal-free QD.[3]

All these detailed statistical analyses (Fig. 1c) based interesting results will be elaborated.

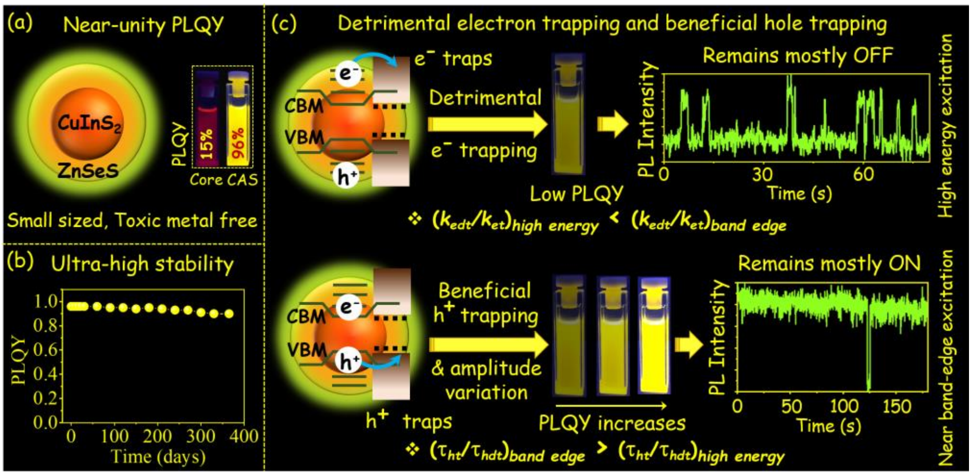

Figure 1. Near-unity PLQY and beneficial intrinsic hole trapping in a toxic metal free CAS QD.

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Unveiling the Interaction Modes of Imiquimod with DNA: Biophysical and Computational Studies

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We report the interaction of an important drug, Imiquimod (IMQ), with Calf Thymus Deoxyribonucleic Acid (ct-DNA).[1] Despite of being used IMQ in multiple medicinal applications such as immune response modifier, antitumor and antiviral drug its interaction with DNA is not studied yet. To understand their interaction and characterize the binding mechanism between groove and intercalation modes, we used various spectroscopic tools. Fluorescence quenching, time-resolved emission, steady state anisotropy technique, ethidium bromide (EtBr), and 4′,6-diamidino-2-phenylindole (DAPI) displacement assays provided us biophysical aspects of IMQ-DNA interactions. All the above studies revealed the binding mode as intercalation mechanism. Circular Dichroism (CD) also well corroborated the intercalation of IMQ into DNA. Thermodynamic parameters of these binding interactions were interpreted with the help of temperature dependent spectroscopic studies characterizing the interaction as enthalpy driven. Further, the binding interactions is explored with the help of molecular docking studies. Based on experimental and computational studies it was concluded that the drug binds to DNA via intercalation mode in AT-rich DNA sequences. These biophysical investigations not only improve our comprehension of IMQ's therapeutic effectiveness but also clarifies the sequence dependent binding processes underlying comparable drug-DNA interactions.

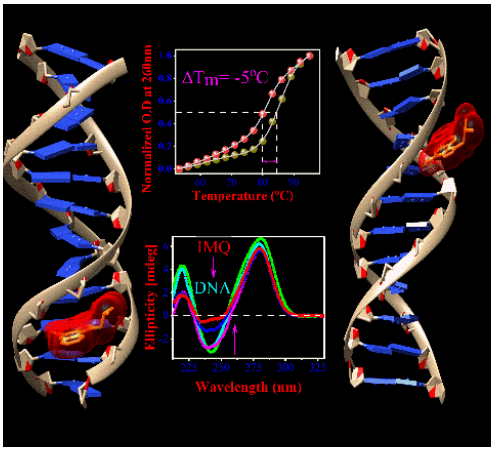

Figure 1. Graphical abstract.

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A Water-Soluble Conjugated Polyelectrolyte for Selective and Sensitive Detection of Carcinogenic Chromium (VI)

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Environmental water pollution caused by hexavalent chromium (Cr (VI)) is a threat to living beings due to its carcinogenic nature. Herein, we report the synthesis of a highly fluorescent water-soluble conjugated polyelectrolyte PPMI and its application as a fluorescence sensor to monitor traces of carcinogenic Cr (VI) ions in water. PPMI was synthesized via the oxidative polymerization method followed by post-polymer functionalization. Fluorescent PPMI exhibited a photoluminescence quantum yield of 23.87 and displayed a rapid, very selective, and sensitive turn-off fluorescence signal in response to Cr (VI), with a significantly high quenching constant of 1.32 × 106 M^{-1}. The mechanism of sensing was found to be static quenching. The limit of detection of this highly accessible analytical method was found to be in nanomolar ranges, i.e. 0.85 nM. Additionally, sensing on solid platforms such as economical paper strips was successfully achieved, which is very challenging and highly recommended for any reliable, portable, and economical analytical method.

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Unraveling the Dynamics and Microheterogeneity of Deep Eutectic Solvents: Insights from Spectroscopy and Molecular Simulations

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Deep eutectic solvents (DESs) constitute a blend of hydrogen bond donors (HBD) and hydrogen bond acceptors (HBA) in specific molar ratios, resulting in a melting temperature lower than that of individual components. These versatile viscous fluids have found diverse applications across various domains. The formation of spatially heterogeneous nano-domains in DESs, attributed to intricate hydrogen bond interactions, underscores the pivotal role of viscosity in their dynamics. In this study, we scrutinize the spectral diffusion and orientational relaxation dynamics through two-dimensional infrared spectroscopy and molecular dynamics simulations. Our comparative analysis emphasizes the profound impact of inter-component hydrogen bond dynamics within HBD and HBA, offering valuable insights into domain-specific microheterogeneity within DESs. By manipulating the hydrogen bond donors (diol-dicarboxylic acid) and adjusting the molar composition of HBD and HBA, we investigate the evolution of microheterogeneity within DESs. Furthermore, we explore the influence of a cosolvent, such as water, on DESs, elucidating the overall fluctuation dynamics sensed by the vibrational probe and revealing the disruption of hydrogen bond networks in these heterogeneous nanodomains.

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Formation of Cu_2SnS_3 and Cu_2SnSe_3 Nanoparticles via Cation Exchange

Ushita Roy[a], Trupthi Devaiah C[a], Soheil Ershadrad[b], Dipankar Saha[c], Biplab Sanyal[b], Pralay K. Santra*[a]

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In the recent past, ternary chalcogenide nanocrystals, mostly from earth-abundant elements, have been used in various applications, e.g., photovoltaics, photodetector, etc., due to their low band gap and high absorption coefficients. However, the growth of such nanocrystals is complicated and not explored in detail. The complexity arises due to the presence of two different metal ions in the system that have different reactivities towards the chalcogen, and most of the time, binary chalcogenide nanocrystals are formed at the beginning, followed by cation exchange to form the ternary chalcogenide nanocrystals finally.[1]

In this context, we have studied the growth mechanism of Cu_2SnS_3 and Cu_2SnSe_3 nanocrystals via different experimental approaches.[2,3] We found the formation of hexagonal CuS/CuSe followed by Sn incorporation via the disulfide/diselenide bond breaking. This leads to the breaking of the CuS/CuSe nanoplatelets to form the smaller size Cu_2SnS_3 and Cu_2SnSe_3 nanocrystals. We investigated the detailed energetics of the Sn incorporation from theoretical calculations.

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Visible-Light Photocatalysis with Surface-Engineered Nanoparticles

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At the core of any catalysis lies the favorable and tunable catalyst–reactant interactions that are crucial to achieving high yield and desired product selectivity. NPs have cemented a special place in photocatalysis because of their unique optoelectronic properties. The ligands on the surface of NPs can bring various interparticle forces into action, which can directly regulate the catalyst–reactant interactions. However, ligands hold a bad reputation and are responsible for catalyst's surface poisoning. Asking the question of outplaying ligand poisoning while retaining the ligands on NP surface turned out to be pivotal not only in overcoming ligand poisoning but also in regulating the catalytic activities of NPs. Inspired by the actions of enzymes, we developed a strategy based on the fine control of interparticle forces emanating from the surface ligands. The precise tuning of interactions between the NP surface and the reactants helps to channel the reactants toward the NP surface, thereby increasing the local concentration and, hence, the efficiency of catalytic reaction (overcoming ligand poisoning). The proof of concept was demonstrated by exploring the regulation of electrostatic forces in important and challenging NP-catalyzed reactions under visible-light irradiation.

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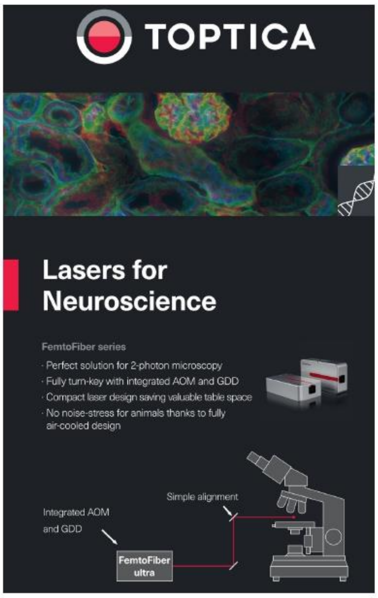

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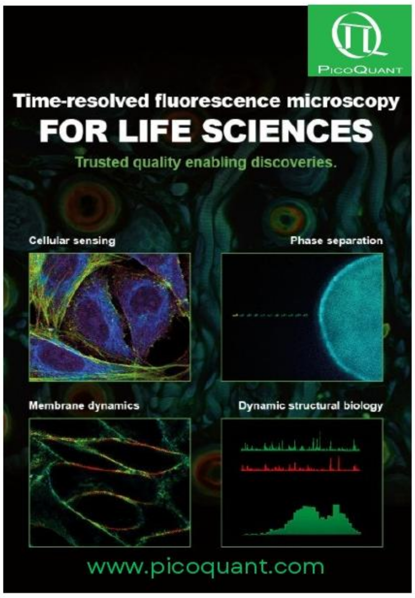

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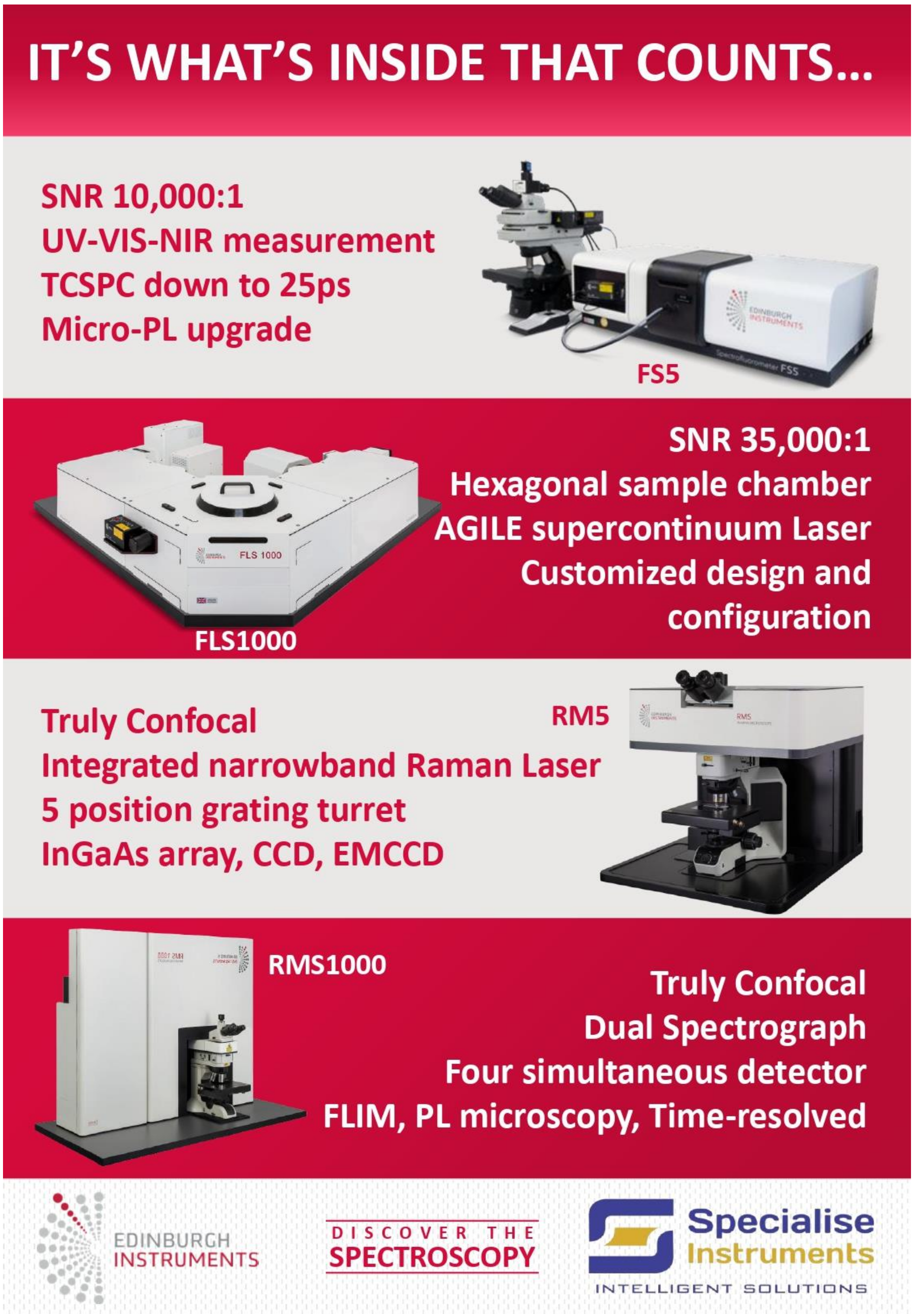

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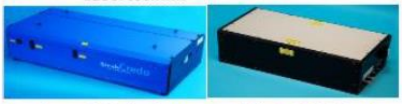
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