SAIS Symposium 2022

Organized by: School of Applied and Interdisciplinary Sciences

Venue: C V Raman Hall, Indian Association for the Cultivation of Science, Kolkata

Date: March 25-26, 2022

Program Schedule

Day 1 (March 25, 2022) FRIDAY

Inaugural Session 10.15 – 10.25 am: Inaugural Address- **Prof. S. Sengupta, IACS** 10.25 – 10.30 am: Welcome Address-Chairman, SAIS, IACS			
Session 1: Chair- **Prof. Pradyut Ghosh**			
Speaker	**Affiliation**	**Time**	**Title**
Dr. Santhosh Babu Sukumaran	CSIR- National Chemical Laboratory	10:30 – 11:00 am	**IL1**: *Solvent-free Organic Liquids: A processable Soft Material with Exciting Optical Features.*
Prof. Kaustabh K. Maiti	CSIR-NIIST	11:00 – 11:30 am	**IL2**: *Advancement of Surface Enhanced Raman Spectroscopy in Biomedical Applications.*
Tea Break: 11:30 -11:40 pm			
Session 2: Chair- **Prof. Prasanta K Das**			
Dr. Ritesh Ranjan Pal	School of Biological Sciences, IACS	11:40 – 12:10 pm	**IL3**: *Bacterial Stealthy Straw for Intra- and Inter-kingdom Communication.*
Prof. Joyram Guin	School of Chemical Sciences, IACS	12:10 – 12:40 pm	**IL4**: *Asymmetric Catalysis with N-Heterocyclic Carbene*
Mr. Ujjwal Ghosh	SAIS, IACS	12:40 – 12:55 pm	**SL1**: *Synthesis of Phosphorodiamidate morpholino oligonucleotides (PMO) using Fmoc chemistry*
Mr. Pranay Saha	SAIS, IACS	12:55 – 1:10 pm	**SL2**: *Selective Pathological and Intracellular Detection of Human Serum Albumin Based on Both Photophysical and Electrochemical Means Using a FRET-based Molecular Probe*

Lunch Break: 1:10 -2:30 pm			
Session 3: **Chair- Prof. Suhrit Ghosh**			
Prof. Martin Brinkmann	Institute Charles Sadron, France	2:30 – 3:10 pm	**KN1**: *Controlling Structure and Orientation in Semi-conducting and Conducting Polymer Thin Films*
Dr. Shubhadeep Datta	School of Physical Sciences, IACS	3:10 – 3:40 pm	**IL5**: *Controlling Electrical Signals in Insulators*
Ms. Subhra Nad	SAIS, IACS	3:40 – 3:55 pm	**SL3**: *Naphthalene diimide based Conjugated Polymers for Electrochromic Application*
Ms. Dipanwita Roy	SAIS, IACS	3:55 – 4:10 pm	**SL4**: *Highly Transparent and Flexible Efficient waveguide Fabricated Using Quaternary Copper Cadmium Sulfide Selenide Quantum Dots*
Tea Break: 4:10-4:20 pm			
Session 4: Chair- **Prof. Shyamal K Saha**			
Dr. Anindita Das	SAIS, IACS	4:20 – 4:50 pm	**IL6**: *Controlled Two-Dimensional Architectures of π-Conjugated Chromophores by Crystallization-Driven Polymer Assembly*
Dr. K D M Rao	SAIS, IACS	4:50 – 5:20 pm	**IL7**: *Heterointerfacial engineering for modulating the electronic properties of $Ti_3C_2T_x$ MXene via charge transfer interactions*
Mr. Ranajit Barman	SAIS, IACS	5:20 – 5:35 pm	**SL5**: *Chain-folding Regulated Antibacterial Polymeric Materials*
Mrs. Sharmistha De Dalui	SAIS, IACS	5:35 – 5:50 pm	**SL6**: *Contaminant Binding to Ferrihydrite Nanoclusters: An Electronic Structure Study*
Mr. Mintu Karmakar	SAIS, IACS	5:50 – 6:05 pm	**SL7**: *Jamming and Band Formation by Active Particles with Restricted Self-propulsion*
Dinner: 7.00-10:00 pm			

Day 2: (March 26, 2022) SATURDAY

Speaker	Affiliation	Time	Title
Session 5: Chair- **Prof. Surajit Sinha**			
Prof. Tapas K Maji	JNCASR-Bangaluru	10:00 – 10:40 am	**KN2:** *Coordination Driven Metal-Organic Functional 'Soft' Materials*
Prof. Alakananda Hajra	Visva-Bharati University	10:40 – 11:10 am	**IL8**: *Design, Synthesis, and Functionalization of Imidazoheterocycles*
Tea Break: 11:10-11:20 am			
Session 6: Chair- **Prof. Somobrata Acharya**			
Dr. Dibyendu Das	IISER-Kolkata	11:20 – 11:50 am	**IL9:** *Substrate induced Catalyst Formation under Non-equilibrium Conditions*
Dr. Shinto Varghese	SAIS, IACS	11:50 – 12:20 pm	**IL10**: *Mechanical Conformity in π-Conjugated Molecular Crystals*
Dr. Praveen Kumar	School of Materials Sciences, IACS	12:20 – 12:50 pm	**IL11**: *Hybrid 2D-Material's Heterostructures for Green H2 Generation*
Dr. Anuja Datta	SAIS, IACS	12:50 – 1:20 pm	**IL12**: *Novel Organic and Inorganic-Organic Hybrid Thermoelectric Materials and Versatile Device Fabrication for Efficient Thermal Energy Harvesting*
Vote of Thanks: Dr . K D M Rao 1:20-1:30 pm			
Lunch & Departure			

KN – Keynote Lecture (30 + 10 mins);
IL – Invited Lecture (25 + 5 mins);
SL – Student's Lecture (12 + 3 mins)

In case participants can't make it to the venue
Join Zoom Meeting: **https://zoom.us/j/95628715637**

Meeting ID:**956 2871 5637**
Passcode: **953172**

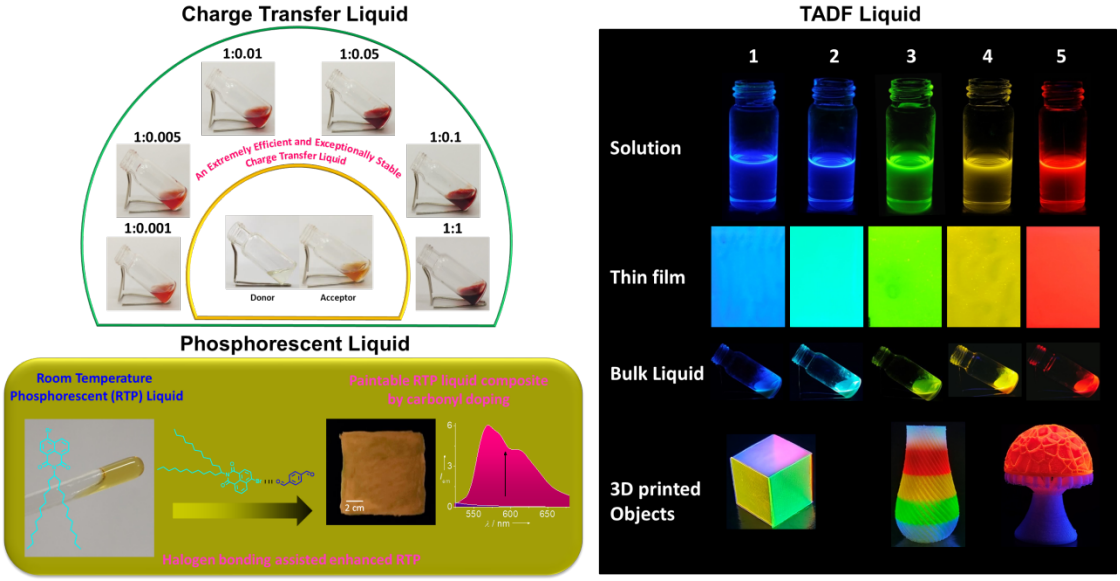
IL1:

Solvent-free Organic Liquids: A processable Soft Material with Exciting Optical Features

Santhosh Babu Sukumaran

Organic Chemistry Division, National Chemical Laboratory (CSIR-NCL),
Dr. Homi Bhabha Road, Pune-411008, India
Email: sb.sukumaran@ncl.res.in

Abstract: Solvent-free organic liquids have been developing as a new soft material parallel to solute-solvent-based systems, where the solvents control the solute molecules exclusively.[1] In molecular systems studying charge transfer, energy/electron transfer, etc., solvent molecules and thereby polarity of the medium creates a drastic difference in the efficiency. Hence to study the ground and excited-state properties of functional chromophores in the absence of solvents, our group extended the research to develop many solvent-free organic liquids that exhibit unprecedented photophysical properties compared to the solid/crystalline analogs. The ground-state donor-acceptor interactions have been modulated to develop a highly stable and efficient charge-transfer liquid at a very low loading of the acceptor; 1 acceptor molecule for 1000 donor molecules.[2] Another study explored the room temperature phosphorescence features of a solvent-free organic liquid phosphor.[3] Two-component luminescent hybrid liquids exhibit synergistic optical properties entirely different from the corresponding solid analogs.[4,5] In a recent development, thermally activated delayed fluorescence of a solvent-free organic liquid exhibiting monomer-like optical features in bulk was investigated.[6] Organic TADF liquids have been used for developing tunable emission hybrid liquids through energy transfer and found helpful in 3D printing applications.



1. Babu, S. S.; *Phys. Chem. Chem. Phys.* **2015**, *17*, 3950-3953; 2. Wakchaure, V. C.; Pillai, L. V.; Goudappagouda, Ranjeesh, K. C.; Chakrabarty, S.; Ravindranathan, S.; Rajamohanan P. R.; Babu, S. S.; *Chem. Commun.* **2019**, *55*, 9371-9374; 3. Goudappagouda, Manthanath, A.; Wakchaure, V. C.; Ranjeesh, K. C.; Das, T.; Vanka, K.; Nakanishi, T.; Babu, S. S.; *Angew. Chem. Int. Ed.* **2019**, *58*, 2284-2288; 4. V. C. Wakchaure, S. D. Veer, A. D. Nidhankar, Goudappagouda, R. Nayak, K. Asokan, S. Ravindranathan, S. S. Babu, *Chem. Commun.* **2022**, *58*, 1998-2001; 5. V. C. Wakchaure, Goudappagouda, T. Das, S. Ravindranathan and S. S. Babu, Nanoscale, 2021, 13, 10780-10784; 6. Nidhankar, A. D., Goudappagouda, Babu, S. S. **2022**, *Unpublished Results*.

IL2:

Advancement of Surface Enhanced Raman Spectroscopy in Biomedical Applications

Kaustabh Kumar Maiti

Principal Scientist, CSTD, Organic Chemistry Section, CSIR-National Institute of Interdisciplinary Science and Technology (NIIST), Industrial Estate P.O., Pappanamcode, Trivandrum 695019, India
E-mail: kkmaiti@niist.res.in

Abstract: Surface-enhanced Raman scattering (SERS) investigated as a highly sensitive spectroscopic modality where the signal intensity of molecular vibration enhanced up to 10^8 –10^{14} folds compare to simple Raman spectra. Multiplexing capability of Raman fingerprints, molecular specificity, high sensitivity and capability to fish out complex biological compositions in molecular level augmented SERS as a potential diagnostic modality in biology and medicine. While assessing all the merits of classical Raman spectroscopy, SERS provides a more sensitive and selective detection and quantification platform. Non-invasive, chemically specific and spatially resolved analysis facilitates the exploration of SERS-based nanoprobes in diagnostic and theranostic applications with improved clinical outcomes compared to the currently available so-called state-of-art technologies. Adequate knowledge on the mechanism and properties of SERS based nanoprobes are inevitable in utilizing the full potential of this modality for biomedical applications. The safety and efficiency of metal nanoparticles and Raman reporters have to be critically evaluated for the successful translation of SERS in to clinics.

On the other hand, advancement of nanotechnology holds great promise for both diagnosis and therapy in a number of communicable and non-communicable diseases including cancer, neurodegenerative disorders and infectious diseases which is coined as nano-theranostics. Exploration of a sensitive diagnostic nanoprobe especially towards the aim of point of care treatment is another challenging task for early and accurate detection of cancer biomarkers which facilitates efficacious therapy by reducing the mortality and morbidity. Recently, we have fabrication of programmable nanoparticles that feature an "on-off" switching transition between fluorescence and SERS for the multiplex detection of lung cancer biomarkers which furnished a semi-quantitative evaluation of biomarkers through both the modalities. In another approach we have developed a gold nanorod (GNR) based theranostic nanoprobe for targeting metastatic melanoma by combining PTT, PDT and chemotherapy along with SERS imaging for the better treatment and effective follow up therapeutic response. We believe that this proof-of-concept will provide a blueprint for the diagnosis and differential staging of cancer into various histological subtypes based on the differential expression of the antigens. We have also developed a SERS based immune-sensor to evaluate the presence of Alzheimer's Disease (AD) biomarker i.e., beta amyloid ($A\beta_{42}$ protein). An efficient SERS based sandwich assay has been successfully demonstrated for an efficient detection of beta amyloid proteins in AD. Therefore, SERS techniques explored as an upcoming molecular diagnostic modality ranging from simple detection platforms to complicated clinical applications.

References:

1. *K.K Maiti et.al.*, **Nano Today**, 2012; 7, 85-93
2. *A N Ramya & K.K Maiti et.al*., **Nanomedicine**., 2015,10(4), 561–571
3. *G Saranya, A. Ajayaghosh, and K. K. Maiti et.al.,* **ACS Applied Materials and Interfaces**, 2018, 10 (45), pp 38807–38818
4. *P. T. Sujai, & K K Maiti** **ACS Applied Biomaterials**, 2019, 2 (1), pp 588–600
5. *M. M. Joseph & K K Maiti et.al.*, **Biomaterials,** 2018, 140-181.

IL3:

Bacterial Stealthy Straw for Intra- and Inter-kingdom Communication

Ritesh Ranjan Pal

School of Biological Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700 032, India,
**E-mail: ritesh.pal@iacs.res.in*

Abstract: Bacteria, the most abundant life-form on earth, reside in a complex multi-species community. They need to maintain intricate molecular crosstalk with proximal prokaryotic and eukaryotic cells to shape their community and flourish in the niche. By infecting host mammalian cells, a Gram-negative pathogenic bacterium enteropathogenic *Escherichia coli* (EPEC) was found to extract nutrients from infected host cell. We termed this phenomenon as host nutrient extraction (HNE). Five inner-membrane proteins coding genes of EPEC pathogenicity island named LEE (locus of enterocyte effacement) were found to be necessary and sufficient for HNE. Coincidentally, these five proteins form a single complex which we named as CORE. The CORE is a known key component of the EPEC injectisome, but for HNE it supports formation of an alternative structure i.e. membranous nanotubes, protruding from the EPEC surface to directly contact the host. The membranous nanotube in bacteria was first reported in a Gram-positive bacterium *Bacillus subtilis* and this conduit was found to be involved in molecular trading between bacteria (BMT, bacterial molecular trading). However, Gram-positive bacteria do not have injectisome but they have the evolutionarily related structure of flagellum. Interestingly, both injectisome and flagella contain highly conserved COREs. We found that lack of COREs resulted in abolition nanotube formation in bacteria. Remarkably, CORE complexes of diverse ancestries, could rescue HNE or MT capacity in native CORE deficient EPEC or *B. subtilis* respectively. Altogether, the results suggest that the CORE is a ubiquitous platform for biogenesis of injectisome, flagella as well as nanotube apparatus in bacteria and the nanotubes help them to conduct contact-dependent exchange of molecules in intra- and inter-kingdom manner.

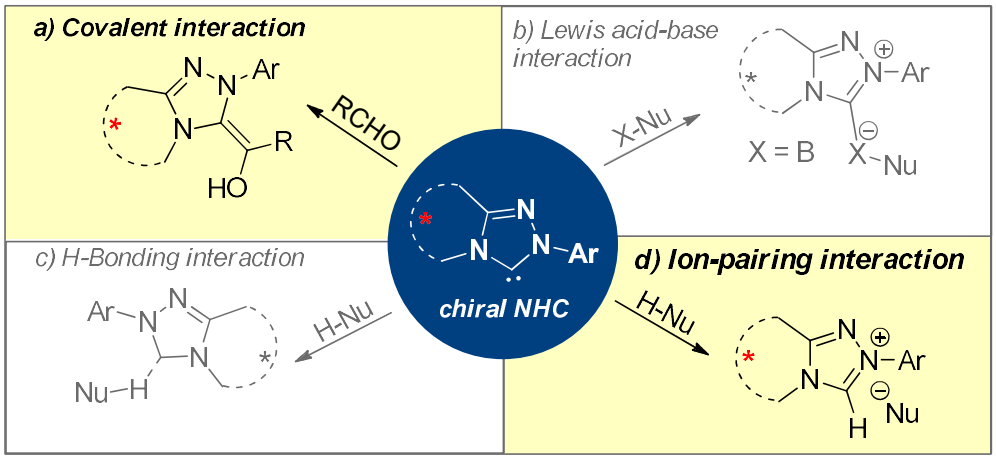
IL4:

Asymmetric Catalysis with *N*-Heterocyclic Carbene

Joyram Guin

School of Chemical Sciences, Indian Association for the Cultivation of Science (IACS)
Kolkata – 700032, INDIA. E – mail: ocjg@iacs.res.in

Abstract: In the domain of asymmetric organocatalyst, chiral N-heterocyclic carbenes (NHCs) have received significant interest. The ability of NHC to activate a diverse class of substrates via different modes of interaction is particularly intriguing.[1] Accordingly, asymmetric NHC-catalysis involving covalent interaction with substrates possessing activated carbonyl functional group, Lewis acid-base interaction with silicon or boron reagents and hydrogen bonding interaction with the substrates in the presence of a proton shuttle[4] have been developed. Furthermore, attempts have also been made in developing asymmetric NHC-catalysis via ion-pairing interaction with substrates utilizing the intrinsic Brønsted base characteristic of NHCs without having much success. Our group is actively working on the development of novel enantioselective organic transformations using NHC-catalysis via covalent as well as ion-pairing interaction with substrates. Some recent findings [2] of our group on asymmetric NHC-catalysis will be discussed during the lecture.



References:

1. (a) D. M. Flanigan, F. Romanov-Michailidis, N. A. White and T. Rovis, *Chem. Rev.*, **2015**, *115*, 9307; (b) M. N. Hopkinson, C. Richter, M. Schedler and F. Glorius, *Nature*, **2014**, *510*, 485.
2. (a) A. Porey, B. D. Mondal and J. Guin, *Angew. Chem. Int. Ed.* **2021**, *60*, 8786; (b) S. Santra, A. Porey, B. Jana and J. Guin, *Chem. Sci.*, **2018**, *9*, 6446; (c) A. Porey, S. Santra and J. Guin, *J. Org. Chem.*, **2019**, *84*, 5313; (d) S. Santra, U. Maji and J. Guin, *Org. Lett.*, **2020**, *22*, 468.

SL1:

Synthesis of Phosphorodiamidatemorpholino oligonucleotides (PMO) using Fmoc chemistry

Ujjwal Ghosh and Surajit Sinha

School of Applied & Interdisciplinary Sciences
Indian Association for the Cultivation of Science
Jadavpur, Kolkata-700 032
Email: camdr@iacs.res.in

Abstract: Phosphorodiamidatemorpholino oligonucleotides (PMO) are routinely used for gene silencing and the recently developed PMO-based drug "Exondys51" has highlighted the importance of PMO as excellent antisense reagents. However, the synthesis of PMO has remained challenging.

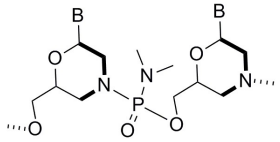


Figure 1: Structure of PMO

Here a method for the synthesis of PMO using Fmoc-protected active morpholino monomers using chlorophosphoramidate chemistry in the presence of a suitable coupling agent on a solid support has been presented. After screening several coupling agents (tetrazole, 1,2,4-triazole, ETT, iodine, LiBr and dicyanoimidazole), ETT was found to be suitable for efficient coupling. Fmoc chemistry was not known for PMO synthesis because the preparation of Fmoc-protected chlorophosphoramidate monomers was not trivial. Synthesis of Fmoc-protected activated monomers and their use in PMO synthesis is reported for the first time. 25-mer PMO has been synthesized and validated *in vivo* in the zebrafish model by targeting the *no tail* gene. Methods have been transferred in DNA synthesizer which has become user friendly for PMO synthesis and opened a new avenue to explore PMO for various applications.

SL2:

Selective Pathological and Intracellular Detection of Human Serum Albumin Based on Both Photophysical and Electrochemical Means Using a FRET-based Molecular Probe

Pranay Saha and Santanu Bhattacharya
School of Applied & Interdisciplinary Sciences
Indian Association for the Cultivation of Science
Jadavpur, Kolkata-700 032

Abstract
Proper diagnosis linked to appropriate medication nowadays has become an essential step in addressing any clinical manifestation. Most diagnostic steps have become largely dependent on complex array-based protocols or sophisticated instrumental techniques. Biochemical sensors can lead to proper disclosure of a particular diseased condition at a relatively low cost in a high-throughput way. Fabrication of new and progressive biosensors is challenging due to their specific design leading to decisive and accurate results.
The most abundant and important protein in blood plasma is human serum albumin (HSA). HSA levels differ in various biological samples and vary widely with different clinical conditions, making HSA an important marker for monitoring different diseased conditions. Therefore, measuring HSA levels in bio-fluids like urine, blood plasma, pleural fluid, cerebrospinal fluid, etc., is mandatory in afflicted patients.
A simple, easily synthesizable, low-cost, fluorescent turn-on probe has been developed for the selective and quantitative detection of human serum albumin (HSA) in different biological fluids collected from patients with various clinical manifestations. The sensor can detect HSA levels by both photophysical and electrochemical means. It is also efficient in rapidly quantifying HSA levels in single living cells, lysates, and tissue extracts with high sensitivity. Higher (millimolar) and trace (micromolar) amounts of serum albumin can be accurately quantified using this probe in a vast array of biomedical samples. This chemical sensor can also be used as a part of Förster Resonance Energy Transfer (FRET) based system adding further accuracy to the measurement technique. Intracellular concentrations of HSA can be measured as well as imaged using this newly synthesized probe. Electrochemical detection of HSA concentrations can also be achieved with this biosensor using a potentiostat. Thus, this probe offers a unique potential of diagnosing HSA levels directly in various biological samples, using its bimodal (i.e., photophysical and electrochemical) properties.

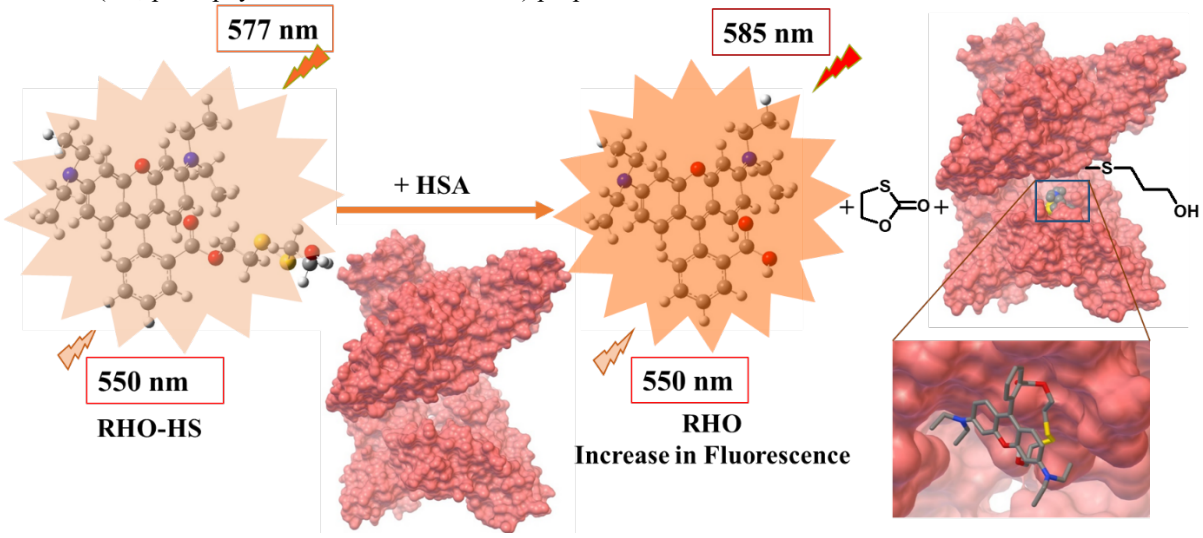


Figure 1. Schematic representation on the working principle of the bio-sensor. The Figure depicts the chemical reaction between the synthesized probe (RHO-HS) and human serum albumin (HSA).

KN1 :

Controlling Structure and Orientation in Semi-conducting and Conducting Polymer Thin Films

Martin Brinkmann

Institute Charles Sadron CNRS, Université de Strasbourg, Strasbourg 67034, France

Abstract: This contribution focuses on recent advances in growth control and oriented crystallization of semi-conducting and conducting polymers. We present representative results related to the orientation of polymer semiconductors using epitaxy and high-temperature rubbing. High-T rubbing is an effective alignment method to orient a large palette of polymer semiconductors (PSCs) with n- or p-type character without alignment substrate. The concurrent roles of the polymer molecular weight distribution and the rubbing temperature (TR) on the in-plane orientation are highlighted. Correlations are drawn between nanomorphology and crystallinity on one side and charge transport and optical properties on the other side. Simple sequential doping using oxidant molecules such as F4TCNQ and F6 TCNNQ help transform semi-conducting oriented PSCs into conducting ones. High anisotropy of optical and electronic properties is thus observed. For instance, charge conductivity and thermopower can both be enhanced along the rubbing direction, leading to remarkable improvement of the thermoelectric power factor of doped films. In this contribution, we focus on two archetypical polythiophenes e.g. poly(2,5-bis(3-dodecyl-2-yl)thieno[3,2-b]thiophene) (C12-pBTTT) and regioregular poly(3-hexylthiophene) (P3HT) doped with different molecular dopants. Charge conductivities up to 2·10^5 S/cm and metallic-like thermopowers similar to iodine-doped polyacetylene are obtained. Doped aligned polythiophene films are almost optically transparent in the visible range and show strongly polarized near-infra-red polaronic bands (dichroic ratio > 10). Dopants are intercalated in the layers of alkyl side chains causing an expansion of the unit cell along the side chains and a contraction along the pi-stacking direction. The extent of lattice expansion is a function of dopant geometry, concentration and side chain length/packing. We demonstrate that he aligned liquid- crystal-like structure of C12 -PBTTT is essential to reach high charge conductivities contrary to the semi-crystalline morphology of P3HT.

References:

(a) A. Hamidi Sakr et al., Adv. Funct. Mat. 2016, 26, 408.
(b) A. Hamidi-Sakr, et al, Adv. Funct. Mat. 2017, 1700173
(c) V. Vijayakumar et al. Adv. Energy Mat. 2019, 27, 1900266.
(d) Y. Untilova et al. Macromolecules 2020, 53, 2441
(e) V. Untilova et al. Macromolecules 2021, 54, 6073
(f) P. Durand et al. Adv. Energy Mat. 2022, 12, 2103049

IL5:

Controlling Electrical Signals in Insulators

Subhadeep Datta

School of Physical Sciences, Indian Association for the Cultivation of Science,
2A&B Raja S. C. Mullick Road, Jadavpur, Kolkata – 700032, India

Abstract: The variation of electrical conductivity between an insulator (10^{-22} Ω^{-1} cm^{-1}) and a metal (10^{9} $\Omega^{-1}cm^{-1}$), probably the widest (factor of 10^{31}) for any physical property, lies in how the electrons fill in the allowed bands. The simple distinguishing probe could be applying a voltage difference across a good insulator which would result in negligible electrical current (showing OL in the "resistance" panel of digital multimeter). But to ascertain this observation, we suppose that the electric field is not strong enough to disrupt the electronic structure. However, that might be very crucial when we are dealing with atomically flat graphene-like two-dimensional (2D) objects. Moreover, atomically sharp edge of an insulating 2D material may possibly offer a 1D conducting channel depending on the unavoidable defects (self-interstitial) or substitutional dopants. In this talk, I shall discuss our recent results on spatially correlated electrical current on the stacking boundaries of pristine and doped hexagonal boron nitride (2D insulator) to distinguish from its insulating bulk via conductive atomic force microscopy (CAFM) [1]. While the pristine edges of hBN show an insulating nature, the O-doped edges reveal a current 2 orders higher even for bulk layers where the direct transmission through tunnel barrier is implausible. In addition, while rubbing the edge during scanning in the contact mode, triboelectrification effect (friction induced charge transfer) at the tip–sample contact area may convert an insulating channel into a conducting channel, which in turn can be useful for efficient energy harvesting.

Reference:

[1] B. Das et al. *ACS Nano* **15**(12), 20203–20213 (2021).

SL3:

Naphthalene diimide based Conjugated Polymers for Electrochromic Application

Subhra Nad and Sudip Malik

School of Applied and Interdisciplinary Sciences,
Indian Association for the Cultivation of Science,
2A & 2B Raja S. C. Mullick Road, Jadavpur,
Kolkata – 700032, India, E-mail: psusn2@iacs.res.in

Abstract: NDI derivatives decorated at the diimines possess the classic electronic properties of the p scaffold in optoelectronic materials. Through incorporation with defined p-conjugated D–A connectors, ideal redox performance and electrochromic properties can be achieved in the NDI derivatives. Generally, due to the electron deficiency of the NDI moiety, miscellaneous heteroatom doping on the naphthalene core can effectively change the energy level of highest occupied molecular orbitals (HOMOs) and the lowest unoccupied molecular orbitals (LUMOs) which in turn endows the NDIs with the conceived charge transfer (CT) effect ensuing improved optical and electrical performances. A novel core-substituted naphthalene diimide derivatives capped with electroactive triphenylamine was employed as an electroactive precursor to prepare polymer films through in situ electropolymerization on ITO substrates. In three electrode configuration, reversible multiple colour changes occurred through anodic oxidation and cathodic reduction with relatively good response times, optical contrast, switching stabilities, and coloration efficiencies. The long EC memory as well as high colouration efficiency compared to other TPA based conjugated polymers ensure the potentiality of the polymer films as an efficient EC material for modern display technology.

Reference:

1. H. F. Higginbotham, M. Czichy, B. K. Sharma, A. M. Shaikh,R. M. Kamble and P. Data, Electrochim. Acta, 2018, 273, 264–272.
2. J. Wang, J. Liu, M. Hu, J. Zeng, Y. Mu, Y. Guo, J. Yu, X. Ma,Y. Qiu and Y. Huang, J. Mater. Chem. A, 2018, 6, 11113–11118.
3. S. Nad, S. Malik (manuscript under review).
4. S. Nad, S. Malik, ChemElectroChem, 2020, **7**, 4144–4152.

SL4:

Highly Transparent and Flexible Efficient waveguide Fabricated Using Quaternary Copper Cadmium Sulfide Selenide Quantum Dots

Dipanwita Roy and Somobrata Acharya

School of Applied & Interdisciplinary Sciences
Indian Association for the Cultivation of Science
Jadavpur, Kolkata-700 032
Email: camdr@iacs.res.in

Abstract: Stokes shift engineering of quantum dots is an attractive approach to enhance luminescence efficiency by reducing reabsorption losses. This large Stokes shift leads to minimum reabsorption, a feature beneficial to obtain bright photoluminescence. Here we use a newly designed I–II–VI2 copper cadmium sulfide selenide quantum dots with high photoluminescence quantum yield of ~62 % with extended coverage of the solar spectrum to realize first quaternary quantum dots-based waveguide. A large Stokes shift of 670 meV between the absorption and photoluminescence peaks ensures a suppressed non-radiative reabsorption loss. By impregnating the quantum dots into polydimethylsiloxane, we designed waveguide with average visible transmittance of 70 % without significant deviation of efficiency. The waveguides are highly flexible showing identical photoluminescence efficiencies over a wide range of bending angles up to 110°. Our approach to obtain an unprecedented combination of a large Stokes shift and a high photoluminescence quantum yield illustrates the potential of quaternary quantum dots for meeting the requirements of reliable, sustainable and competitive modulated light guiding systems.

IL6:

Controlled Two-Dimensional Architectures of π-Conjugated Chromophores by Crystallization-Driven Polymer Assembly

Anindita Das

School of Applied and Interdisciplinary Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata-700032, India
Email: (psuad2@iacs.res.in)

Abstract: Crystallization-driven self-assembly (CDSA)[1] of semicrystalline block copolymers (BCPs) has recently emerged as a powerful technique for fabrication of diverse hierarchical anisotropic structures, including two-dimensional (2D) architectures in solutions. In this work, we have utilized the known crystallization property of a biodegradable and biocompatible polymer, i.e., poly(L-lactide) for controlled 2D assembly of distinct π-conjugated chromophores. Poly(L-lactide)s, end-functionalized with dipolar chromophores such as merocyanine (MC) or naphthalene monoimide (NMI) and nonpolar pyrene (PY) or benzene (Bn) crystallize into precise diamond-shaped 2D platelets in isopropanol (iPrOH) under suitable condition, which forces the terminally attached π-systems to assemble on the platelet surface by either dipole-dipole interactions[2] (for NMI and MC) or aromatic stacking (for PY and Bn). This confers exciting photophysical properties to the 2D platelets. Our results reveal that controlled 2D assembly of the end-capped functional chromophores is a consequence of the CDSA of the polymer chain. However, the polarity of the dye plays a critical role in imparting colloidal stability to the 2D platelets in the crystallizable solvent. Further, co-crystallization between NMI- and PY-functionalized poly(L-lactide)s yielded two-component co-platelets of identical shape and structural precision with highly efficient (~80%) Förster Resonance Energy Transfer (FRET) from the donor (PY) to the acceptor (NMI). In contrast, 1:1 mixture of their pre-formed homo-aggregates exhibit no FRET due to narcissistic self-sorting. Moreover, "living" crystallization-driven self-assembly strategy enabled fabrication of hierarchical segmented block co-platelets with sequence-controlled compartmentalized location of the two self-assembled chromophores on the platelet surface. The multifaceted strategy opens up new possibilities for construction of functional 2D architectures with the structural precision of single crystals, which will be the topic of this oral presentation.

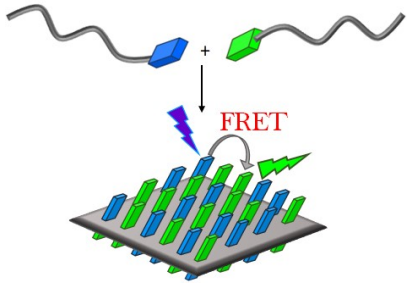


Figure 1. Two-dimensional organization of functional π-systems by crystallization-driven self-assembly of poly(L-lactides).

References:

1. L. MacFarlane, C. Zhao, J. Cai, H. Qiu, I. Manners, *Chem. Sci.* **2021**, *12*, 4661.
2. S. Ganda, M. H. Stenzel, *Prog. Polym. Sci,* **2020**, *101*, 101195.
3. F. Würthner, *Acc. Chem. Res.* **2016**, *49*, 868.
4. A. Rajak, A. Das, *Angew. Chem. Int. Ed.* **2022**, doi.org/10.1002/anie.202116572.

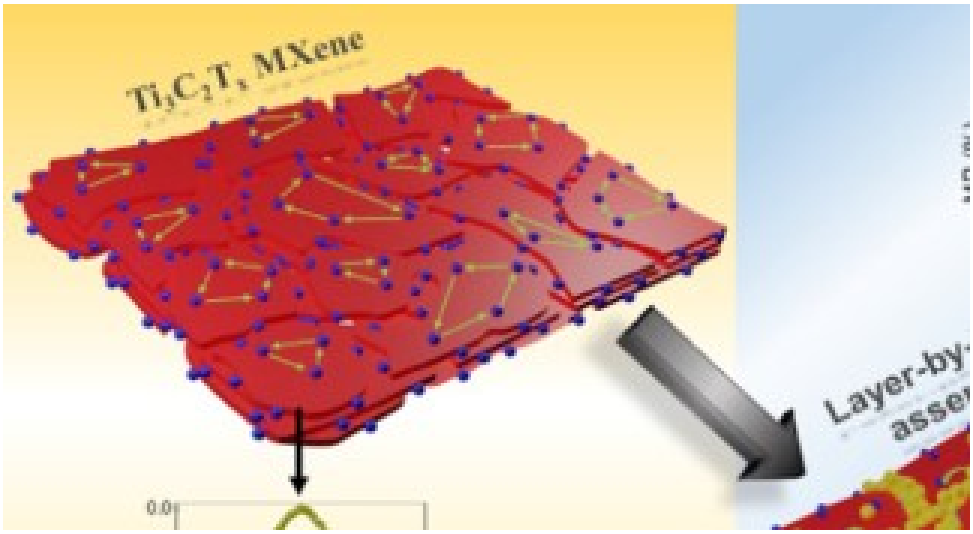
IL7:

Heterointerfacial engineering for modulating the electronic properties of $Ti_3C_2T_x$ MXene via charge transfer interactions

K D M Rao

School of Applied and Interdisciplinary Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata-700032, India
Email: (saiskdmrao@iacs.res.in)

Abstract: Two-dimensional (2D) transition-metal carbides (MXenes) are emerging as promising materials for a wide range of applications owing to their intriguing electrical, optical, and optoelectronic properties. However, the modulation of metallic $Ti_3C_2T_x$ MXene electronic properties is the key challenge to fabricate functional nanoelectronic devices. Here, I would like to talk about heterointerfacial engineering $Ti_3C_2T_x$ MXene/CuI nanoparticle by employing a layer-by-layer assembly process. The charge transfer at the heterointerfacial assembly is monitored qualitatively from the quenched photoluminescence emission of CuI. The stable electrical conductivity and consistent Raman spectra of the 3-LBL assembly (three sequential stacks of CuI/MXene) signify the oxidation stability of $Ti_3C_2T_x$ thin films even after exposure to the ambient environment for 2 months. Furthermore, the 3-LBL assembly exhibited a three-dimensional (3D) variable-range hopping-based electrical conduction in the temperature range $2 \leq T < 100$ K, contrary to the weak localized transport phenomenon in $Ti_3C_2T_x$ MXene. Therefore, the modulated electrical transport and superior oxidation stability of the $Ti_3C_2T_x$ MXene in the 3-LBL assembly have the potential to develop next-generation optoelectronic and memory devices.



Reference:

[1] K Karmakar, P Sarkar, J Sultana, N Kurra, and KDM Rao - ACS Applied Materials & Interfaces, 2021.

SL5:

Chain-folding Regulated Antibacterial Polymeric Materials

Ranajit Barman and and Suhrit Ghosh

Senior Research Fellow, School of Applied and Interdisciplinary Sciences
Indian Association for the Cultivation of Science, 2A and 2B Raja S. C. Mullick Road, Kolkata, India-700032
Email- psurb3@iacs.res.in

Abstract: Despite a rapid growth in cationic host defence peptide (CHDP)-mimicking synthetic antibacterial polymers, the importance of the well-defined secondary structure of the synthetic polymers similar to CHDP has not been studied in context of bacterial membrane perturbation. Recently we have investigated series of cationic amphiphilic alternating polyurethanes (PUs) for antibacterial activity with specific focus on the effect of chain folding on the antibacterial activity. Some of them contain linear flexible hydrocarbons (F-PUs) while others contain cyclic rigid hydrocarbons (R-PUs) in the segmented polymers backbone. F-PUs exhibit Intra-chain H-bonding driven pleated structure followed by hierarchical assembly, producing cationic polymersome in water. In sharp contrast, R-PUs, deprived of the chain-folding possibility due to the rigid linker, exhibit immiscibility driven aggregation producing spherical particles. F-PUs exhibit exemplary antibacterial activity with exceptionally low minimum inhibitory concentration (MIC), while R-PUs do not show even moderate activity. Beyond planktonic bacteria, F-PUs also exhibit extraordinary biofilm eradication efficiency. This presentation will focus on the chain-folding regulated self-assembly and antibacterial activity of these newly developed alternating amphiphilic PUs.

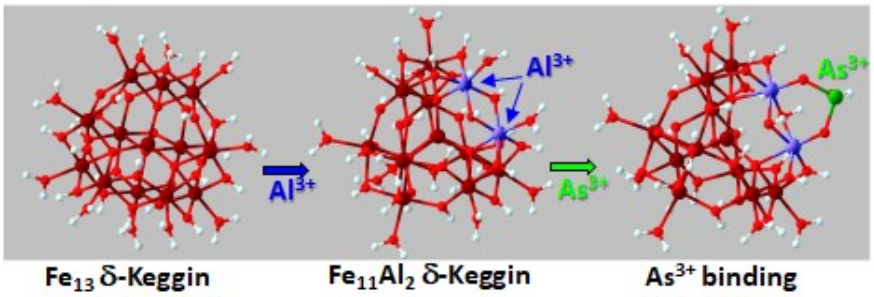
SL6:

Contaminant Binding to Ferrihydrite Nanoclusters: An Electronic Structure Study

Sharmistha De Dalui and Bidisa Das

School of Applied and Interdisciplinary Sciences (SAIS)
Indian Association for the Cultivation of Science. Jadavpur. Kolkata.

Abstract: Ferrihydrite is a naturally occurring nanostructured mineral abundantly found in the environment.[1]Immense surface reactivity of ferrihydrite nanoparticles plays a very important role in the transformation and mobility of contaminants/pollutants in the environment.[2] We use density functional theory (DFT) to model ferrihydrite nanoclusters in their formative stages and study the binding of contaminant ions like arsenite and arsenate in water.[3,4]We consider small ferrihydrite nanoclusters like dimers, trimers and the δ-Fe_{13} Keggin clusters of gradually increasing size in a "bottom-up"molecular approach to model the contaminant binding. We compare the binding free energies of the contaminant ions to ferrihydrite nanoclusters as they increase in size to form larger multinuclear clusters.[4]We also look into the effect of Aluminum doping in ferrihydrite nanoclusters to study how the arsenic binding potential is affected by impurity ions. The calculated reaction free energies clearly show that Al doping into ferrihydrite clusters reduce their As^{3+} binding potential, whereas, the As^{5+} binding is not affected much due to Aldoping.[4]



References:

1. Michel, F. M.; Ehm, L.; Antao, S. M.; Lee, P. L.; Chupas, P. J.; Liu, G.; Strongin, D. R.; Schoonen, M. A. A.; Phillips, B. L.; Parise, J. B. *The Structure of Ferrihydrite, a Nanocrystalline Material.Science,* **2007***, 316,* 1726-1729.
2. Johnston, C. P.; Chrysochoou , M. *Mechanisms of Chromate, Selenate, and Sulfate Adsorption on AlSubstituted Ferrihydrite: Implications for Ferrihydrite Surface Structure and Reactivity, Environ. Sci. Technol., **2016**,* 50, *3589–3596.*
3. Das, B. *Theoretical study of small iron–oxyhydroxide clusters and formation of ferrihydrite.J. Phys. Chem A.*,**2018,** *122,* 652-661.
4. DeDalui, S.; Das, B. *Binding of As^{3+} and As^{5+} to Fe(III) Oxyhydroxide Clusters and the Influence of Aluminum Substitution: A Molecular Perspective.J. Phys. Chem. A.,* **2022**, 126, 5, 670–684.

SL7:

Jamming and Band Formation by Active Particles with Restricted Self-propulsion

Mintu Karmakar and Raja Paul

School of Mathematical & Computational Sciences, IACS, Kolkata

Abstract: Nonequilibrium statistical physics is particularly interested in the study of systems with persistent energy consumption and dissipation at the scale of the constituent particles. By classifying such systems as active matter, we can gain a better understanding of the phenomenon of autonomous collective movement in the living world known as flocking. The flocking transition is an out-of-equilibrium phenomenon that occurs frequently in nature,ranging from human crowds, mammalian herds, bird flocks, and fish schools to unicellular organisms such as amoebae, bacteria, collective cell migration in dense tissues, and sub-cellular structures such as cytoskeletal filaments and molecular motors. In this presentation, I will introduce the active matter paradigm, briefly remember some early work, review recent results on single-particle and collective behaviour, and suggest future directions.

KN2:

Coordination Driven Metal-Organic Functional 'Soft' Materials

Tapas Kumar Maji

Molecular Materials Laboratory, Chemistry and Physics of Materials Unit, School of Advanced Materials (SAMat), Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore-560064
E-mail: tmaji@jncasr.ac.in; Web: www.jncasr.ac.in/tmaji

Abstract: Nanoscale processable soft organic-inorganic hybrid materials find several applications in biological and material sciences.[1] In general such materials is built by the self-assembly of low molecular weight gelators (LWMG) based linker and metal ions.[1]The inclusion of metal ions into low molecular weight gelator systems has proven to be advantageous in combining the functionality of traditional coordination chemistry with a wide array of exciting applications.[2] Here novel and interesting optical, electronic, magnetic and catalytic properties can be introduced based on synergistic interactions of metal ions and LWMG. [3-7]Additionally, stimuli-responsive behaviour is just another reason that such soft material will reside at the forefront of chemical technology. These soft hybrids can also be exploited in energy and environmental applications, like the photo or electro-catalytic water splitting, CO_2 reduction, water purification, or separation and delivery of small molecules.[7-10]
In my talk, I will focus on the rational design and synthesis of several LWMG and their self-assembly with metal ions towards novel functional hybrid soft nano-catalyst materials.

References:

1. Sutar, P.; Maji, T. K. *Chem. Commun.,* **2016**, *52*, 8055
2. Sutar, P.; Surech, V. M.; Jayaramulu, K.; Hazra, A.; Maji, T. K. *Nature Commun.* **2018**, *9*, 3587
3. Roy, S.; Samanta, D.; Kumar, P.; Maji, T. K.; *Chem. Commun.* **2018**, *54*, 275
4. Sutar, P.; Maji, T. K. *Inorg. Chem*. **2017**, *56*, 9417
5. Sutar, P.; Maji, T. K. Maji, *Chem. Commun*. **2016**, *52*, 13136
6. Suresh, V. M.; De, A.; Maji, T. K. C*hem. Commun.* **2015**, *51*, 14678
7. Sutar, P.; Suresh, V. M.; Maji, T. K. *Chem. Commun.* **2015**, *51*, 9876
8. Verma, P.; Singh A.; Rahimi, F.A.; Maji, T. K. *J. Mater. Chem. A*., **2021** 09, 13608
9. Verma, P.; Singh A.; Maji, T. K. *Chem. Sci*., **2021**, 12, 2674
10. Verma, P.; Singh A.; Rahimi, F.A.; Sarkar, P.; Nath, S.; Pati, S. K.; Maji, T. K. *Nature Commun.* **2021,** 12, 7313

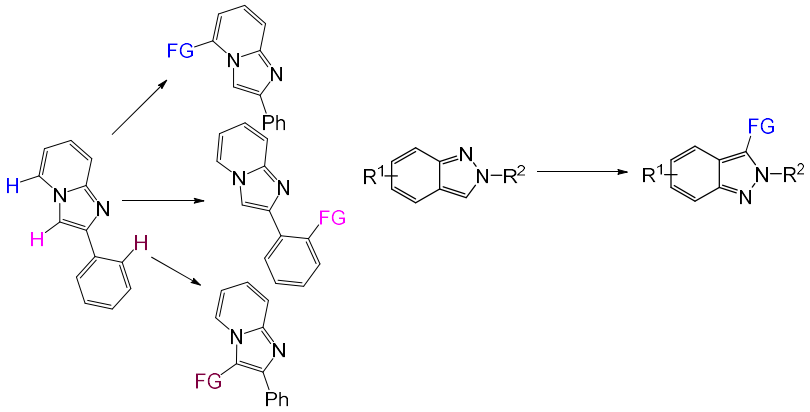
IL8:

Design, Synthesis, and Functionalization of Imidazoheterocycles

Alakananda Hajra

Associate Professor of Chemistry
Visva-Bharati University, West Bengal
E-mail: alakananda.hajra@visva-bharati.ac.in

Abstract: Heterocyclic compounds have gained a great deal of attention as majority of the drugs contain heterocycle scaffolds. So the developments of new synthetic strategies for heterocycles are prime targets of the organic chemists over the years. Imidazopyridine is one of the important fused bicyclic 5–6 heterocycles and it is recognized as "drug prejudice" scaffold due to its wide applications in medicinal chemistry. This scaffold is the constituent of various marketed drug like zolpidem, alpidem, zolimidine, necopidem, saripidem etc. Recently, visible-light photocatalysis has become an impressive tool in organic synthesis. In this realm, the merger of transition metal catalysis and visible light photoredox catalysis offers an exciting opportunity to perform the organic transformations in mild conditions. In this lecture I will discuss our recent works on sustainable synthesis of imidazo[1,2-*a*] pyridines,[1,2] and indazoles[3]



Scheme 1. Regioselective functionalization of imidazopyridine and indazole

References and Notes:

1. (a) Bagdi, A. K.; Santra, S.; Monir, K; Hajra, A. *Chem. Commun.* **2015,** *51***,** 1555.
2. (a) Mitra, S.; Hajra, A. *Org. Lett.* **2014,** *16,* 5652; (b) Mishra, S.; Monir, K.; Mitra, S.; Hajra, A. *Org. Lett.* **2014,** 16, 6084; (c) Mondal, S.; Hajra, A. *Org. Lett.* **2017,** *19,* 3751; (d) Samanta, S.; Mondal, S.; Ghosh, D.; Hajra, A. *Org. Lett.* **2019,** *21,* 4905.; (e) Singsardar, M.; Mondal, S.; Laru, S. Hajra, A. *Org. Lett.* **2019,** *21,* 5606.
3. (a) Ghosh, P.; Mondal, S.; Hajra, A. *Org. Lett*. **2020**, *22*, 1086; (b) Neogi, S.; Ghosh, A. K.; Majhi, K.; Samant, S.; Kibriya, G.; Hajra, A. *Org. Lett.* **2020**, *22*, 5605; (c) Bhattacharjee, S.; Laru, S.; Hajra, A. *Chem. Commun.* **2022**, *58*, 981.

IL9:

Substrate induced Catalyst Formation under Non-equilibrium Conditions

Dibyendu Das

Dept of Chemical Sciences and CAFM,
IISER Kolkata
(e-mail:dasd@iiserkol.ac.in)

Abstract: There remain critical gaps in our understanding of the emergence of functional biopolymers in the origins of Earth's biosphere. For instance, extant proteins, evolved over millions of years, carry out an impressive array of responsibilities, from catalysis and molecular recognition to motility and compartmentalization. One of the major goals of our lab is to investigate the possible origins of advanced enzymatic functions from folds of short peptide based paracrystalline phases. Further, we are excited about understanding the non-equilibrium structures of living systems.[1-6] I will show our recent discoveries of simple chemical systems that can be substrate-driven to access higher energy self-assembled states, just as seen in natural microtubules. Further, I will attempt to sketch our aims of developing self-assembled autonomous materials that can show temporal control of functions.[5,7-10]

References and Notes:

1. S.P. Afrose, C. Mahato, P. Sharma, L. Roy, and D. Das*. J. Am. Chem. Soc. 2022, (Just Accepted)
2. S. Pal, A. Reja, S. Bal, B. Tikader and D. Das* Angew. Chem. Int. Ed. 2022, (Just Accepted)
3. A. Chatterjee, C. Mahato and D.Das* Angew. Chem. Int. Ed. 2021, 60, 204-209
4. B. Sarkhel, A. Chatterjee and D. Das*. J. Am. Chem. Soc. 2020 142 4098-4103
5. Reja, S.P. Afrose, D. Das*. Angew. Chem. Int. Ed. 2020 59 4329-4334
6. S. Bal, C. Ghosh, T. Ghosh, R. Vijayaraghavan and D. Das*. Angew. Chem. Int. Ed. 2020, 59, 13506
7. S.P.Afrose, S. Bal, A. Chatterjee, K. Das, D. Das* Angew. Chem. Int. Ed. 2019 58 15783-1578
8. S. Ahmed, A. Chatterjee, K. Das and D.Das* Chemical Science 2019 10 7574-7578
9. S. Bal, K. Das, S. Ahmed and D.Das* Angew. Chem. Int. Ed. 2019 58 244
10. H. S. Azevedo, S. L. Perry, P. A. Korevaar, D. Das. Nature Chemistry 2020, 12, 793-794

IL10:

Mechanical Conformity in π-Conjugated Molecular Crystals

Shinto Varghese

School of Applied and Interdisciplinary Sciences
Indian Association for the Cultivation of Sciences

Abstract: Flexible optoelectronics emerged as the need of the hour due to increasing demand for wearable and conformable devices. The key requirement of these devices is to withstand mechanical deformations without compromise in device performance. Crystalline organic π-conjugated molecules as active materials can offer an enhanced performance due to their superior charge and exciton transport properties over the semi-crystalline/amorphous counterparts. Organic molecular crystals are generally brittle and shattered into pieces on subject to subtle mechanical perturbation, which limit its application. A greater part of the fragile nature arises from the anisotropic packing of molecules in the crystal lattice, where the applied force dissipated in an asymmetric manner along the molecular planes resulted in the rapture of the three-dimensional network. Seminal research work commenced by different groups brought about the consensus that the isotropic dissipation of applied stress is the key towards the mechanical compliance of the crystals. In a large variety of systems, the bending ability is due to a) interactions topology acting in the orthogonal directions b) corrugated structures and buffering weak and dispersive interactions and c) structural isotropy. However, most of the observations on mechanically compliant crystalline materials are serendipitous in nature. A more intense research is required to derive a rule of thumb design concepts to develop crystalline materials with mechanical compliances. Diverse structural motifs and synergetic interactions reported in the available literature that governs the mechanical compliances to applied stress in single crystals, untangling and differentiating the precise aspects responsible for mechanical conformity remains a major challenge. In my talk, I will be discussing our efforts in these directions on a few optoelectronically relevant molecular structures and our strategies to fine tune the molecular packing for mechanical conformity. [1]

Reference:

[1] M. Ghora, P. Majumdar, M. Anas, S. Varghese , Chem. Eur. J. **2021**, *26*, 14488-14495.

IL11:

Hybrid 2D-Material's Heterostructures for Green H_2 Generation

Praveen Kumar

School of Materials Science, Indian Association for the Cultivation of Science, Kolkata -700032, India
Email: praiitr@gmail.com, praveen.kumar@iacs.res.in

Abstract: Photoelectrochemical splitting of water into hydrogen and oxygen has been accepted as a sustainable way to utilize solar energy. Among several photoactive materials, 2D-Materials connected *via* van der Waals forces have gained tremendous attention as competent material for PEC HER as the most stable 2H phase (of MoS_2) possesses good catalytic property comparable to noble metal, suitable band edge position, appropriate energy bandgap, and photochemical stability. Having all these salient features, 2D materials are still not being utilized to their maximum possibility for PEC HER due to the lack of an alternative way of basal plane activation. Further, growing vertical heterostructures of these 2D-materials on foreign substrates like GaN, Si is also one of the prime concerns to increase the active surface area and promote efficient charge separation & transport. In my talk, I will address some of these issues and also will discuss related successful recent innovations in our laboratory.

References:

1. ACS Journal of Physical Chemistry Letters 13 (2022) 1334.
2. Chemical Engineering Journal 435 (2022) 134963.
3. Nano Energy 87 (2021) 106119
4. Renewable & Sustainable Energy Reviews 135 (2021) 110391.
5. ACS Applied Materials & Interfaces 12 (2020) 28792
6. ACS Applied Materials & Interfaces 12 (2020) 37218
7. ACS Applied Energy Materials 3 (2020) 6834
8. Chemical Engineering Journal 397 (2020) 125415.
9. ACS Applied Materials & Interfaces, 12 (2020) 13797.
10. Nature Communications Chemistry 2 (2019) 4.

IL12:

Novel Organic and Inorganic-Organic Hybrid Thermoelectric Materials and Versatile Device Fabrication for Efficient Thermal Energy Harvesting

Anuja Datta

School of Applied & Interdisciplinary Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700 032, India
*E-mail: pusad4@iacs.res.in

Abstract: The increasing alternate energy requirement have encouraged the search for efficient technologies that could be mixed sustainably with renewable energy sources. Moreover, with the increasing global reliance on smart electronic devices and gadgets; self-powered micro-energy sources have now become a necessary choice. In this scenario, thermoelectric (TE) materials are unique part of the solution towards a more energy efficient future and are now routinely adopted for clean, efficient micro-power generation and for solid-state cooling applications.[1,2] Organic thermoelectric materials (OTEs) and hybrid Organic-Inorganic TE materials systems, in spite of their low-performances, are finding niche applications in internet-of-things, wearable wireless, and smart health monitoring devices, due to their flexibility, robustness and low cost. Conducting polymers because of their intrinsic low thermal conductivity, and general non-toxicity are popular choice in OTEs.[1,3,4] By tuning the electrical conductivity (n-type by doping donor and p-type by doping acceptor molecules) and by enhancing Seebeck coefficient in conducting polymer-inorganic TE hybrid materials systems, efficient thermal energy harvesting devices may be generated.[3,4] Whilst choice for p-type OTEs are widespread (PEDOT:PSS, PANI etc.), there is still lack for stable (in air) n-type OTE materials.

We recently investigated an amphiphile derivative of naphthalene-diimides (cNDI-1), that indicated promising negative Seebeck value (S ~ -237μV/K) from the pristine NDI molecule. NDI due to the presence of the electron deficient aromatic ring with a planar structure, are one of the most promising electron-deficient building blocks to construct air-stable n-type semiconducting devices, which I will discuss in the talk. Another aspect of exploring hybrid TE materials systems for energy applications lies in exploring versatile and cost-effective device fabrication processing. In this direction, I will present as how simple pencil tracing and pressing even on Xerox and Emery papers using different Organic-Inorganic hybrid TE materials systems (PEDOT:PSS-Graphite and PEDOT:PSS-Bismuth) might prove to be reliable and efficient way of scavenging thermal energies from surrounding heat.

References:

1. Russ B. et al. Nat Rev Mater., 2016, 1, 16050.
2. Datta A. et al. (a) "Nanostructuring in Anisotropic Low Temperature Thermoelectric Materials" in Thermoelectric Nanomaterials, Eds, Springer Series in Materials Science, Springer, 2013. (b) CRC Handbook on Thermoelectrics and Its Energy Harvesting on Materials, Preparation and Characterization, 2012.
3. Bubnova et al. Energy Environ. Sci., 2012, 5, 9345.
4. Mondal et al. Chem. Nano. Mat., 2022, 8, e202100367.