

DEPARTMENT OF **CHEMICAL SCIENCES**



2023

Messages from the Director's and Head's Desk



I am delighted that the IISER Mohali Department of Chemical Sciences is releasing an updated departmental brochure in 2023. The Department of Chemical Sciences has expanded steadily over recent years from a young department that was established in 2012 to currently a department with twenty-five faculty members. The department's research portfolios cover a wide range of chemistry, from the conventional areas of organic, inorganic, and physical chemistry to the more cutting-edge fields of green chemistry, nanotechnology, and theoretical chemistry. Some of the faculty are also working on multidisciplinary projects that combine chemistry with biology, physics, and materials science. The various fundamental and advanced ideas in chemistry are covered in teaching courses for BS-MS, Int-PhD, and PhD students. The department is amongst the foremost in India's chemical sciences research community. The combined efforts of committed faculty members, motivated students, and dedicated support staff have made this possible. The faculty members and students published a significant number of research articles and granted patents and have received several honors and awards. I wish everyone of the department's PhD and BS-MS students, research associates, lab personnel, and faculty members tremendous success in their future academic efforts. May they continue to bring the institute many honors in the years to come.

J. Gowrishankar
Director, IISER Mohali



The Department of Chemical Sciences, established in June 2012, is one of the six Departments of IISER Mohali. The Department offers courses in chemistry for BS-MS, Int. PhD and PhD programs of the Institute. Doctoral and post-doctoral research work is carried out in all major areas of chemical and allied sciences. The Department offers a conducive atmosphere to students and faculty to foster the spirit of scientific inquiry and to pursue cutting-edge research. Major thrust is in the contemporary areas of inorganic & organometallics, solid state & materials chemistry, organic synthesis, catalysis, chemical biology, polymers, molecular recognition, NMR methodology, X-ray crystallography, theoretical chemistry, computer simulations and energy, environment & sustainability. The Department houses a state-of-the-art instrumentation facility, funded by the Institute and external funding agencies, to facilitate research work in these areas. The Department has a dedicated team of qualified staff members and distinguished faculty, trained at renowned Institutes in India and abroad. The faculty members attract substantial financial support from government and private agencies for their research activities. Several members of the faculty have received prestigious honors in the form of fellowships, medals/prizes for distinction in their areas of research. The faculty have been active in organizing scientific meetings from time to time and have also been invited to deliver lectures at various national and international forums, conferences, and symposia. We are proud of our alumni who have shined in their further chosen career paths and contribute to the betterment of society by contributing to industry and academia all over the world. Currently, the department has about 100 registered PhD and Int. PhD students working in the above focus areas. In the coming years, the department looks forward to engaging in applied research and technology development through engagement in industrial projects.

Sanjay Singh
Head of the Department

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Sanjay K. Mandal
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Inorganic Chemistry, Nano Science and X-ray Crystallography

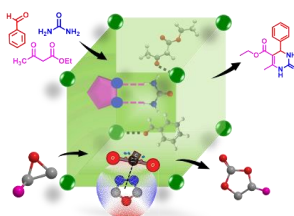
Profile:

Prof. Mandal received his B. Sc. (with honours) and M. Sc. degrees in Chemistry from the University of Calcutta and IIT Kanpur, respectively. He earned a Ph.D. in Chemistry under the guidance of Professor F. Albert Cotton at Texas A&M University, College Station, USA. In addition to furthering his research skills in academia for next 5 years, he spent about 11 years working in several companies, such as General Electric Company, Dow Corning Corporation, Occidental Chemical Corporation, and Clariant Corporation. He joined IISER Mohali in August 2008 as one of few senior faculty members, established the central X-ray facility, and contributed academically and administratively for the growth of the Institute.

Research Interests:

Prof. Mandal's group is engaged in developing diversified chemistry of elements across the periodic table through a variety of interdisciplinary projects that involve multi-step organic synthesis, coordination chemistry, catalysis and materials chemistry. Various spectroscopic techniques (UV-vis, FTIR, NMR, Raman, CD and Fluorescence), thermal analysis (TGA and DSC), electrochemistry, surface analysis (SEM/EDX, AFM and TEM), and X-ray crystallography (PXRD and SCXRD) are routinely used for establishing physicochemical properties of the new organic, inorganic and organometallic compounds. This has resulted in the strategic design of porous materials with a special emphasis on Metal Organic Frameworks (MOFs) and Covalent Organic Frameworks (COFs) for their diverse structural aesthetics and for their possible roles in various applications, such as catalysis, molecular separation, gas and liquid adsorption.

luminescence, gas and liquid adsorption, magnetism, etc. The major projects that we work on are: (i) design of bifunctional heterogeneous catalysts with hydrogen-bond-donating (primary amide group) and/or hydrogen-bond-accepting (oxadiazole moiety) capabilities along with Lewis acid centers for numerous organic transformations, and (ii) development of multifarious micro- and mesoporous nanomaterials for (a) sequestration and conversion of carbon dioxide, (b) ultrafast/selective sensing of metal ions and neutral small molecules (nitro-aromatics and ketones) at ppb/ppt level, and (c) study of non-radioactive surrogates of nuclear wastes such as multimedia I₂ capture and selective sensing of ReO₄⁻ in water, and (iii) fabrication of metal oxides and sulfides for photocatalysis, luminescence, and organic transformations.



Heterogeneous Catalysis in porous MOFs.

Selected Publications:

(1) "Exploiting a Multi-Responsive Oxadiazole Moiety in One Three-Dimensional Metal-Organic Framework for Remedies to Three Environmental Issues", Alisha Gogia, Himanshi Bhambri and Sanjay K. Mandal, *ACS Appl. Mater. Interfaces*, **2023**, 15, 8241–8252.

(2) "Topologically Driven Pore/Surface Engineering in a Recyclable Microporous Metal-Organic Vessel Decorated with Hydrogen-Bond Acceptors for Solvent-Free Heterogeneous Catalysis", Alisha Gogia and Sanjay K. Mandal, *ACS Appl. Mater. Interfaces*, **2022**, 14, 27941–27954.

(3) "Nitrogen-rich covalent organic frameworks: a promising class of sensory materials", Himanshi Bhambri, Sadhika Khullar, Sakshi and Sanjay K. Mandal, *Materials Advances*, **2022**, 3, 19-124.

(4) "Modulation of hydrophilicity inside the cavity of molecular rectangles self-assembled under ambient conditions", Sadhika Khullar and Sanjay K. Mandal, *Chem. Commun.*, **2020**, 56, 7913-7916.

(5) Design of a Primary-Amide-Functionalized Highly Efficient and Recyclable Hydrogen-Bond-Donating Heterogeneous Catalyst for the Friedel-Crafts Alkylation of Indoles with β -Nitrostyrenes", Datta Markad and Sanjay K. Mandal. *ACS Catalysis*, **2019**, 9, 3165.

(6) "In-Depth Experimental and Computational Investigations for Remarkable Gas/Vapor Sorption, Selectivity, and Affinity by a Porous Nitrogen-Rich Covalent Organic Framework", Prasenjit Das and Sanjay K. Mandal, *Chem. Mater.*, **2019**, 31, 1584.

(7) "A highly emissive fluorescent Zn-MOF: molecular decoding strategies for solvents and trace detection of dunnite in water", Prasenjit Das and Sanjay K. Mandal, *J. Mat. Chem. A*, **2018**, 6, 21274.



From left: Vishnu, Vandana, Sumedha, Himanshi, Prof. Mandal, Babita, Alokandanda, Rupinder, Ishfaq

Samrat Mukhopadhyay

Professor

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Biological Chemistry: Intrinsically Disordered Proteins

Profile:

Ph.D. – 2000-2004/Indian Institute of Science, Bangalore

Visiting Fellow – 2004-05/Tata Institute of Fundamental Research, Mumbai

Postdoc – 2005-2008/The Scripps Research Institute, La Jolla, California, USA

Professional experience – 2008-13/Assistant Professor, IISER Mohali

2013-20/Associate Professor, IISER Mohali

2020-present/Professor, IISER Mohali

He is also a professor in the Department of Biological Sciences at IISER Mohali

In our lab, we utilize a diverse array of tools and concepts from physical chemistry to chemical biology to biophysics and molecular biology to study the intriguing behavior of IDPs. Our efforts are aimed at delineating the fundamental molecular mechanism by which liquid-like condensates are formed and dissipated. We are also studying the liquid-to-solid phase transition into amyloid-like aggregates that are associated with deadly neurodegenerative diseases such as Alzheimer's, amyotrophic lateral sclerosis (ALS), and so forth.

Research Interests:

The overarching goal of our lab is to investigate a wide range of fascinating aspects of intrinsically disordered proteins/regions (IDPs/IDRs) that undergo liquid-liquid phase separation (LLPS) and amyloid formation. IDPs challenge the tenets of the traditional structure-function paradigm and exist as a rapidly interconverting conformational ensemble rather than a single well-defined structure. The conformational plasticity allows them to adopt different structures depending on their binding partners. Therefore, a single polypeptide sequence is capable of accomplishing a range of functions. It is proposed that retaining disorder is an evolutionary strategy that allows complex functions within a compact genome of higher organisms. Additionally, the dysfunction of many IDPs is associated with a range of deadly diseases such as Alzheimer's and Parkinson's diseases and cancers.

Selected Publications:

1. "Heterotypic electrostatic interactions control complex phase separation of tau and prion into multiphasic condensates and co-aggregates" S. K. Rai, R. Khanna, A. Avni & S. Mukhopadhyay* *Proc. Natl. Acad. Sci.* (2023) 120, e2216338120.
2. "Molecular Origin of Internal Friction in Intrinsically Disordered Proteins" D. Das* & S. Mukhopadhyay* *Acc. Chem. Res.* (2022), 55, 3470-3480.
3. "Single-Droplet Surface-Enhanced Raman Scattering Decodes the Molecular Determinants of Liquid-Liquid Phase Separation" A. Avni, A. Joshi, A. Walimbe, S. G. Pattanashetty & S. Mukhopadhyay* *Nature Communications* (2022), 13, 4378.
4. "Sub-stoichiometric Hsp104 regulates the genesis and persistence of self-replicable amyloid seeds of Sup35 prion domain" S. Mahapatra, A. Sarbahi, P. Madhu... S. Mukhopadhyay* *J. Biol. Chem.* (2022) 298, 102143.
5. "Spatiotemporal Modulations in Heterotypic Condensates of Prion and α -Synuclein Control Phase Transitions and Amyloid Conversion" A. Agarwal, L. Arora, S.K. Rai, A. Avni & S. Mukhopadhyay* *Nature Communications* (2022) 13, 1154.
6. "Short-Range Backbone Dihedral Rotations Modulate Internal Friction in Intrinsically Disordered Proteins" D. Das, L. Arora & S. Mukhopadhyay* *J. Am. Chem. Soc.* (2022) 144, 1739-1747.
7. "An intrinsically disordered pathological prion variant Y145Stop converts into self-seeding amyloids via liquid-liquid phase separation" A. Agarwal, S.K. Rai, A. Avni & S. Mukhopadhyay* *Proc. Natl. Acad. Sci.* (2021) 118, e2100968118.
8. "Intermolecular Charge-Transfer Modulates Liquid-Liquid Phase Separation and Liquid-to-Solid Maturation of an Intrinsically Disordered pH-Responsive Domain" P. Dogra, A. Joshi, A. Majumdar & S. Mukhopadhyay* *J. Am. Chem. Soc.* (2019) 141, 20380-20389.



Sanjay Singh
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Organometallic & Macrocyclic Chemistry

Profile:

PhD – 2003-06/University of Göttingen, Germany /Prof. Herbert W. Roesky

Postdoc–2006-2007/University of Göttingen, Germany and University of Cambridge, U.K.

Professional experience – 2008-16

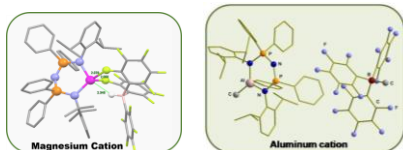
Assistant Professor, IISER Mohali

2016-2022 Associate Professor, IISER Mohali

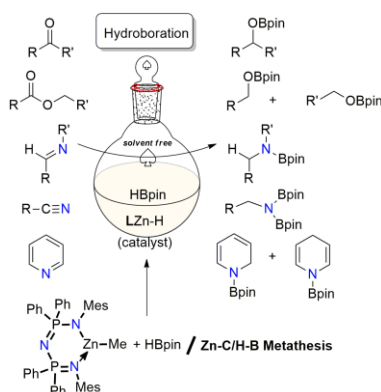
2022-present Professor, IISER Mohali

Research Interests:

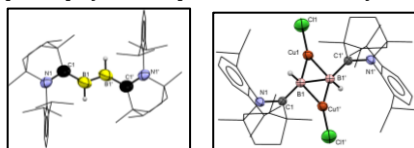
(1) Chemistry of main group and Zn cations: Potent Lewis acidic catalysts



Synthesis of highly Lewis acidic low coordinated cationic complexes of Mg, B, Al and Zn supported by bulky ligands with N_2P or N_3P_2 skeleton is the major emphasis of this research project. The newly discovered cationic complexes have turned out to be highly efficient catalysts for hydroelementation reactions. In the case of Zn complexes even the covalent complexes were sufficiently Lewis acidic to promote hydroboration of various unsaturated substrates (as shown below).

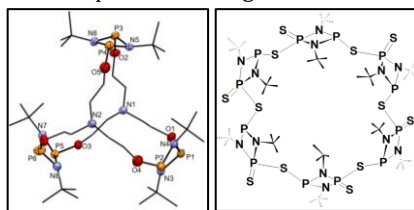


(2) BICAAC and CAAC carbenes as ligands: Low valent species (radicals or zero-valent compounds) are of great interests due to their unique electronic structure and high reactivity. Often, these species require kinetic stabilization by the supporting ligand. We exploit strong donor behaviour of CAAC and BICAAC carbenes to stabilize complexes of low valent transition metals and main group elements (Mn, Ni, Cu, B, Si, P) including investigation of their bonding behaviour, photophysical aspects and reactivity.



(3) Inorganic macrocycles, pyridinophanes and cryptands

Synthesis of phosph(III)azane based macrocycles and cryptands are major theme of this research area. Use of templates in assembling macrocycles and cryptands (shown below) and host-guest chemistry has opened new directions. We are also involved in exploring diarylazo containing phosph(III)azane macrocycle for their photoswitching behaviour.



External Funding:

“Bicyclic(alkyl)(amino) carbene as ligand to support low valent complexes from main group and transition elements and applications thereof in catalysis”

Agency: SERB; 2020-2023

Amount: INR 27,62,100.



Selected Publications:

(1) “Highly Electrophilic Mononuclear Cationic Aluminum Alkoxide Complexes: Syntheses, Reactivity and Catalytic Applications” M. Bhandari, M. Kaur, S. Rawat, S. Singh*, *Chem. Eur. J.*, **2023**, e202301229.

(2) “Hydroboration of Imines and Alkynes Catalyzed by Electronically Unsaturated Aluminum Hydride and Methyl Aluminum Cations” M. Bhandari, M. Kaur, S. Rawat, S. Singh*, *Inorg. Chem.*, **2023**, 62, 6598.

(3) Well-Defined Ni(0) and Ni(II) Complexes of Bicyclic (Alkyl)(Amino)Carbene (MeBICAAC): Catalytic Activity and Mechanistic Insights in Negishi Cross-Coupling Reaction” S. K. Thakur, M. Kaur, K. K. Manar, M. Adhikari, A. R. Choudhury, S. Singh*, *Chem. Eur. J.* **2022**, 28, e202202237.

(4) “Three Coordinated Organoaluminum Cation for Rapid and Selective Cyanosilylation of Carbonyls under Solvent-Free Conditions” S. Rawat, M. Bhandari, B. Prashant, S. Singh*, *ChemCatChem* **2020**, 12, 2407.

(5) “Group 13 Element Containing Conformationally Rigid “N–E–N” Heteroatomic Bridged [3.3](2,6)Pyridinophanes (E = B, Al)” D. Bawari, C. Negi, K. Jaiswal, B. Prashanth, A. R. Choudhury, S. Singh*, *Chem. Commun.*, **2018**, 54, 8857.

(6) “Electronically Unsaturated Three-Coordinate Aluminum Hydride and Organoaluminum Cations.” B. Prashanth, M. Bhandari, S. Ravi, K. R. Shamasundar, S. Singh*, *Chem. Eur. J.* **2018**, 24, 4794.

From Left: Mansi Tanwar, Manu Goyal, Manisha Kumari, Sanjay Singh, Anju Jetia, Soumya Mirdha, Surbhi Bansal, Simranjeet Kaur, Devika G., Gopika R. S., Alisha Sharma.



Ramasamy Vijaya Anand
Professor

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Synthetic Organic Chemistry

Profile:

Ph.D – 1997-2003/IIT Kanpur, UP, India /Prof. Vinod K. Singh

Postdoc – 2004-2005/University of Strathclyde, Glasgow, UK/Prof. John A. Murphy

Postdoc – 2006/Texas A&M University, College Station, USA/Prof. Brian T. Connell

Professional experience – 2006-2009/Scientist/Dr. Reddy's Laboratories Ltd/ Hyderabad/India.

Positions held: 2010-1016/Assistant Professor/IISER Mohali

2016-2022/Associate Professor/IISER Mohali

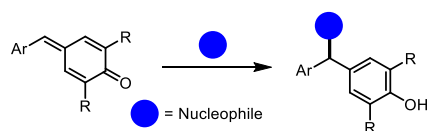
Current Position – Professor (Since November 2022)

Research Interests:

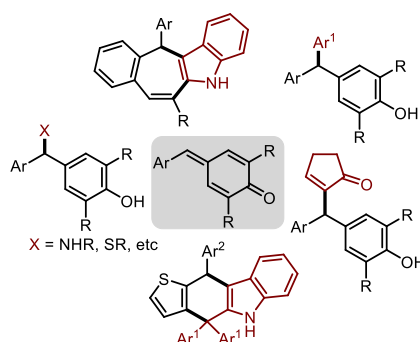
Our group is primarily interested in exploring the synthetic applications of *p*-quinone methides (*p*-QMs). We are also interested in developing organocatalytic transformations using cyclopropenium based small molecules.

(1) *p*-Quinone methides (*p*-QMs) chemistry

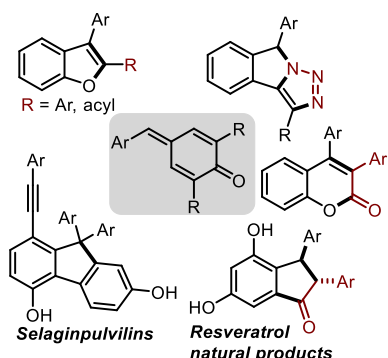
Over the past 7-8 years, our research group is actively involved in the synthetic transformations of *p*-QMs to various useful compounds such as diaryl-/triarylmethanes, carbocycles and heterocycles. In addition, a few appropriately modified *p*-QMs have been utilized as synthons for the total synthesis of biologically active natural products such as (±)-isopaucifloral F, shoreophenol, selaginpulvillins, etc.



(a) Diaryl/triarylmethanes and carbocycles

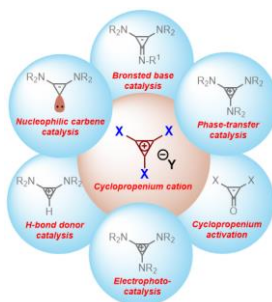


(b) Heterocycles/Natural products



(2) Organocatalysis by cyclopropenium based small molecules

Very recently, we found that the cyclopropenium based salts could be explored as organocatalysts in many fundamental organic transformations.



Selected Publications:

(1) "Pd(II)-Catalyzed Annulation of Terminal Alkynes with 2-Pyridinyl-substituted *p*-Quinone Methides: Direct Access to Indolizines" *Chem. Commun.* **2022**, 58, 13238.

(2) "Construction of Heterocycle-fused Tetrahydrocarbazoles Through a Formal [3+3]-Annulation of 2-Indolylmethanols with *p*-Quinone Methides." *Org. Biomol. Chem.* **2023**, 21, 2493.

(3) "TfOH-catalyzed Intramolecular Annulation of 2-(Aryl)-phenyl-substituted *p*-Quinone Methides Under Continuous-flow: Total Syntheses of Selaginpulvin I and Isoselagintamarlin A" *J. Org. Chem.* **2022**, 87, 3363.

(4) "Bis(amino)cyclopropenium Ion as a Hydrogen-bond Donor Catalyst for 1,6-Conjugate Addition Reactions" *J. Org. Chem.* **2021**, 86, 4994.

(5) "1,6-Hydroolefination and Cascade Cyclization of *p*-Quinone Methides with Styrenes: Total Synthesis of (+/-)-Isopaucifloral" *J. Org. Chem.* **2018**, 83, 10107.

(6) "N-Heterocyclic carbene catalyzed 1,6-conjugate addition of Me₃Si-CN to *para*-quinone methides and fuchsones: Access to α-arylated nitriles" *Org. Lett.* **2017**, 19, 1982.

Group Members



Photo taken in March 2023

Santanu Kumar Pal

Professor

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Supramolecular Chemistry

Profile:

PhD – 2003-08/Raman Research Institute, Bangalore, India

Postdoc – 2008-10/University of Wisconsin, Madison, USA

Professional experience–

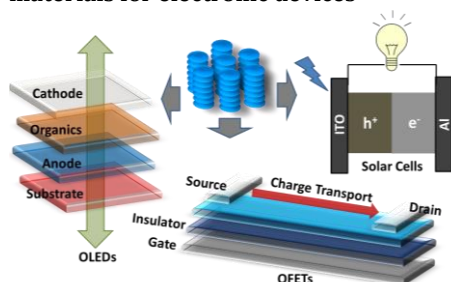
2010- 2016/Assistant Prof. /IISER Mohali.

2016-2022/Associate Prof. /IISER Mohali.

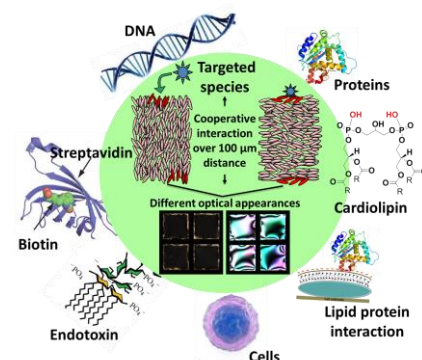
2022-present/Professor /IISER Mohali.

Research Interests:

Liquid Crystal nanocrystals: Functional materials for electronic devices

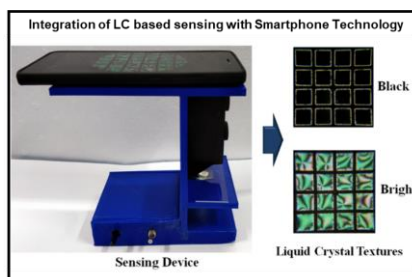


Organic electronic devices have gained increased attention in the field of OLEDs, OFETs and photovoltaics. A promising class of materials in this research field is discotic liquid crystals (DLCs) which exhibit one-dimensional columnar superstructures and therefore, have advantageous properties such as, great processability and modulated self-organization behaviour. We develop materials that fulfil such demands suitable for devices. Another objective is to study and understand the soft self-assembly behaviour of nanoparticles functionalized with organic groups. The aim is to provide a new resource of materials for applications in the nanosciences.



Passive sensor materials based on LCs

Recently, the dynamic and responsive properties of synthetic LCs appear potentially useful to the realization of new classes of sensors and actuators. The realization of this potential, however, requires advances in the engineering of such LC-based stimuli-responsive interfaces. We are interested to the development of new principles which offer the basis of general and facile approaches to the building of new LC-sensing platforms that can report presence/organization of targeted bio- and chemical agents.



Porous Organic Polymers for Sensing and Visible Light Photocatalytic Applications

In this project, our aim is to synthesize various porous organic polymers and covalent organic frameworks for sensing and to tune band gap of the polymers to drive a specific visible-light driven photocatalytic conversion.

Selected Publications:

(1) "Observation of "de Vries-like" properties in bent-core molecules." Kaur, S.; Barthakur, A.; Mohiuddin, G.; Gupta, S. P.; Dhara, S.; Pal, S. K.*, *Chem. Sci.*, **2022**,13, 2249-2257.

(2) Probing Nanoscale Lipid-Protein Interactions at the Interface of Liquid Crystal Droplets. Pani, I.; K. M., F. N.; Sharma, M.*; Pal, S. K.*, *Nano Lett.* **2021**, 11, 4546-4553.

(3) Molecular Engineering for the Development of a Discotic Nematic Mesophase and Solid-State Emitter in Deep-Blue OLEDs. De, J.; Yadav, R. A. K.; Yadav, R. S.; Gupta, S. P.; Joshi, M.; Choudhury, A. R.; Jayakumar, J.; Jou, J. -H.; Cheng, C. -H.; Pal, S. K.*, *J. Org. Chem.*, **2021**, 86, 7256-7262.

(4) High Hole Mobility and Efficient Ambipolar Charge Transport in Heterocoronene-Based Ordered Columnar Discotics. De, J., Bala, I., Gupta, S. P., Pandey, U. K.,* Pal, S. K.*, *J. Am. Chem. Soc.*, **2019**, 141 (47), 18799-18805.

(5) "Room temperature Discotic Liquid Crystalline Triphenylene Pentalkynylbenzene dyads as an emitter in blue OLEDs and their Charge transfer complexes with ambipolar charge transport behaviour" I. Bala, W. Y. Yang, S. P. Gupta, J. De, R. A. K. Yadav, D. P. Singh, D. K. Dubey, J. H. Jou, Redouane Douali, S. K. Pal* *J. Mater. Chem. C*, **2019**, 7, 5724.

(6) "Natural sunlight driven oxidative homocoupling of amines by truxene based conjugated microporous polymer" V. R. Battula, H. Singh, S. Kumar, I. Bala, S. K. Pal*, K. Kailasam *ACS Catal.* **2018**, 8, 6751.

(7) "Observation of polar order and thermochromic behaviour in a chiral bent-core system exhibiting exotic mesophases by superstructural frustration" V. Punjani, G. Mohiuddin, S. Kaur, R. K. Khan, S. Ghosh, S. K. Pal* *Chem. Commun.* **2018**, 54, 3452-3455.

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Chemical Physics and Spectroscopy

Profile:

Ph.D – 1997-2001/IIT Madras, Chennai /Prof. Mangala Sunder Krishnan

Postdoc – 2001-2007/Massachusetts Institute of Technology (MIT), USA /Prof. Robert G Griffin

Professional experience –

2007-2008 –Assistant Professor, IIT Roorkee

2008-2016: Assistant Professor, IISER Mohali

2016-Present: Associate Professor, IISER Mohali

Research Interests:

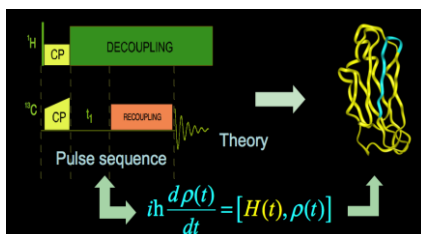
- (a) Theory and Methodology development in solid-state NMR spectroscopy
- (b) Time dependent Quantum mechanics
- (c) NMR Quantum computing in the solid-state.

Solid-state nuclear magnetic resonance (SSNMR) is the application of NMR spectroscopy to systems that are solids, nearly solids, or strongly anisotropic. Recent advancements in this field have established solid-state NMR as a viable alternative for determining the structure of biological systems (membrane proteins and peptide aggregates) that are less amenable to characterization by other high-resolution techniques. In spite of the tremendous progress made in the last decade or so, SSNMR is still a developing field and methods towards structural characterization are just emerging.

The primary objectives of our research group are to invoke the principles of physics and try to apply them in solving problems in chemistry and structural biology. In this regard, we plan to use Solid-state Nuclear

proteins and their role in diseases.

Besides its implications in chemistry and structural biology, SSNMR can also be used as a test-bed to investigate/understand some of the founding principles of quantum physics



Research Publications @ IISERM:

(1) On the exactness of effective Floquet Hamiltonians employed in solid-state NMR spectroscopy, Rajat Garg and Ramesh Ramachandran, *J. Chem. Phys.* **2017**, 146, 184201.

(2) Analytic Theory of Multiple-Quantum NMR of Quadrupolar Nuclei, G. Vinay and R. Ramachandran, *Annual Reports on NMR Spectroscopy*, **2016**, 89, 123.

(3) Unraveling multi-spin effects in rotational resonance NMR using reduced density matrix theory, U. SivaRanjan and Ramesh Ramachandran, *J. Chem. Phys.* **2014**, 140, 054101.

(4) Nuances of Multi-Quantum excitation in solid-state NMR of quadrupolar nuclei, Deepansh Srivastava and Ramesh Ramachandran, *RSC Advances*. **2013**, 3, 25231.

(5) Understanding cross-polarization (CP) NMR experiments through dipolar truncation, Manoj Kumar Pandey, Zeba Qadri and Ramesh Ramachandran, *J. Chem. Phys.* **2013**, 138, 114108.

(6) Understanding multi-quantum NMR through secular approximation, Deepansh Srivastava, R. Venkata SubbaRao and Ramesh Ramachandran, *Phys. Chem. Chem. Phys.* **2013**, 15, 6699.

(7) Concept of effective Hamiltonians for transitions in multi-level systems, R. Venkata SubbaRao, Deepansh Srivastava and Ramesh Ramachandran, *Phys. Chem. Chem. Phys.* **2013**, 15, 2081.

Group members



From left to right (Rajat, Nisha, Ramesh, Shreyan and Vinay)

S. S. V. Rama Sastry
Associate Professor
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Organic Synthesis and Catalysis

Profile

Ph.D – 2001-05/Indian Institute of Science, Bangalore/Prof. A. Srikrishna.

Postdoc – 2005-08/The Scripps Research Institute, California, USA/Prof. Carlos F. Barbas, III.

Professional experience

2008-2010/Biocon-BMS Research Center (BBRC), Bangalore.

2010-11/Jubilant Biosys Ltd, Bangalore.

2011-2017/Assistant Professor, IISER Mohali

2017-till/Associate Professor, IISER Mohali

Research Interests

- Our research primarily focuses on the development of sustainable and atom economic reactions via organophosphine catalysis, palladium-catalyzed allylic alkylation reactions, one-pot cascade transformations employing sulfur ylides, and applying these strategies in the synthesis of bioactive natural products and pharmaceutically important compounds.

- Our research emphasizes on cultivating medicinal chemistry aspects and industry-relevant research.

- The new synthetic methodologies are designed to incorporate the contemporary concepts such as asymmetric synthesis, diversity-oriented approaches, green and sustainable chemistry, step, atom and pot economy, etc.

Our philosophy

Our research philosophy is that the methods we develop should be user-friendly, experimentally trivial, environmentally friendly, and economically sound while providing access to otherwise difficult targets of structural and biological significance.

Our webpages

Find more details about our research activities here:

<https://web.iisermohali.ac.in/faculty/sastry>

<https://www.iisermohali.ac.in/faculty/dcs/ramsastry>

Selected Publications

(1) 'An Interrupted Corey-Chaykovsky Reaction of Designed Azaarenium Salts: Synthesis of Complex Polycyclic Spiro- and Fused Cyclopropanoids' Singh, B.;[#] Ansari, A. J.;[‡] Malik, N.; Ramasastry, S. S. V. *Chem. Sci.* **2023**, *14*, 6963.

(2) 'Pd-Catalyzed Formal [3+3] Annulation of Benzylic *gem*-Diacetates: Synthesis of Various (Hetero)Arene-Fused Benzo[*f*]chromenes' Kumar, P; Nikam, M. M.; Ramasastry, S. S. V. *Organometallics* **2022**, DOI: 10.1021/acs.organomet.2c00472 [*Invited*]

(3) 'Phosphine-Mediated Redox Cyclization of 1-(2-Nitroaryl)prop-2-ynones to 3-Hydroxyquinolin-4-ones: Formal Intramolecular Oxyamination of α,β -Ynones' Dutta, L.; Ramasastry, S. S. V. *Org. Lett.* **2022**, *24*, 7665.

(4) 'Pd-Catalyzed Formal [3+3] Heteroannulation of Allylic *gem*-Diacetates: Synthesis of Chromene-Based Natural Products and Exploration of Photochromic Properties' Kumar, P.; Kumar, P; Venkataramani, S.; Ramasastry, S. S. V. *ACS Catal.* **2022**, *12*, 963.

(5) 'Phosphine-Catalyzed Intramolecular Vinylogous Aldol Reaction of α -Substituted Enones' Mondal, A.; Satpathi, B.; Ramasastry, S. S. V. *Org. Lett.* **2022**, *24*, 256.

(6) 'Annulative Morita-Baylis-Hillman reaction to synthesise chiral dibenzocycloheptanes' Mondal, A.; Shivangi.; Tung, P.; Wagulde, S.; Ramasastry, S. S. V. *Chem. Comm.* **2021**, *57*, 9260.

(7) 'Catalytic Enantioselective Synthesis of Axially Chiral Diarylmethylidene Indanones' Kumar, P.;[#] Shirke, R. P.;[#] Yadav, S.; Ramasastry, S. S. V. *Org. Lett.* **2021**, *23*, 4909.

(8) Palladium-catalysed 5-*endo-trig* allylic (hetero)arylation' Singh, B.;[#] Bankar, S. K.;[#] Kumar, K.; Ramasastry, S. S. V. *Chem. Sci.* **2020**, *11*, 4948.



Sugumar Venkataramani

Associate Professor

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Physical Organic Chemistry

Profile:

Ph.D – 2003-07/Ruhr University

Bochum, Germany/Prof. Wolfram Sander

Postdoc – 2008-09/Christina Albrecht

University Kiel/Alexander von Humboldt

(AvH) fellowship/Prof. Rainer Herges

Professional experience – 2010-13/

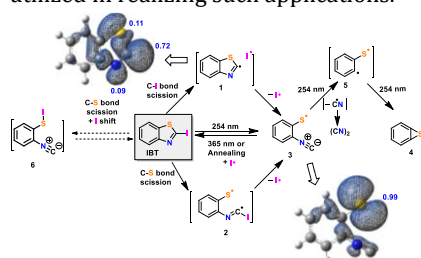
Orchid Pharma, Chennai/Research

Scientist

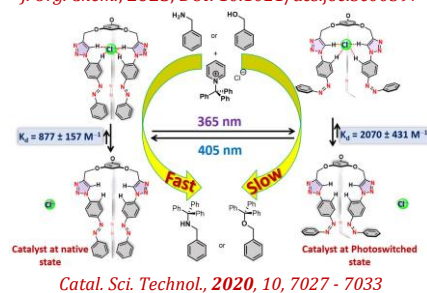
Research Interests:

Photoswitchable and light controllable functional molecules:

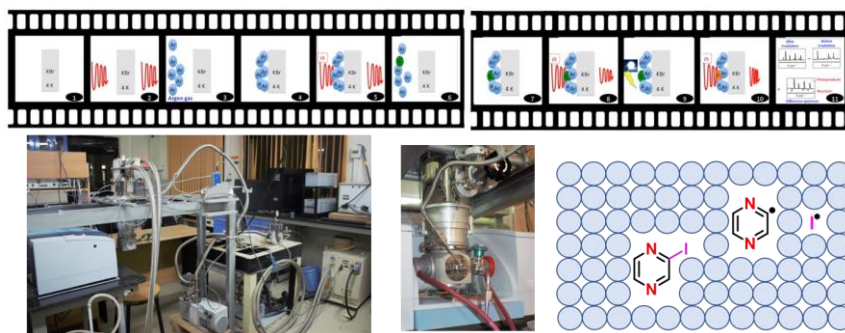
One of our primary interests is to design and develop novel light-controllable azoheteroarene-based photoswitches and molecules containing multiple azo systems. Through interdisciplinary work ranging from synthesis to spectroscopic and microscopic studies, the exploration of fundamental aspects of light-controlled applications, such as encapsulation and release of guest molecules, sensors, and catalysis, are being intended. Physical organic chemistry-based concepts and DFT computations are extensively utilized in realizing such applications.



J. Org. Chem., **2023**, DOI: 10.1021/acs.joc.3c00597



Catal. Sci. Technol., **2020**, *10*, 7027 - 7033



Matrix isolation infrared spectroscopic and computational studies of reactive intermediates and unstable compounds:

Another important goal is understanding the structure, stability and reactivity of radicals and highly reactive intermediates. In this regard, we utilize an experimental technique called matrix isolation infrared spectroscopy. At very low temperatures (4 K), rare gases form transparent matrices in the UV and IR regions. By controlling the dilution in such gases, molecules can indeed be isolated. If the precursors with photolabile groups/atoms are used under photolytic conditions, reactive intermediates can be generated. A detailed spectroscopic investigation will be performed along with computations to understand the electronic structural and reactivity aspects. Studies on heterocyclic transient species are currently underway.

Selected Publications:

(1) "Bistable Aryl Azopyrazolium Ionic Photoswitches in Water" Ankit Kumar Gaur, Debapriya Gupta, Anjali Mahadevan, Pravesh Kumar, Himanshu Kumar, Dhanyaj Narayanan Nampoothiry, Navneet Kaur, Sandeep Kumar Thakur, Sanjay Singh*, Tomáš Slanina*, and Sugumar Venkataramani* *J. Am. Chem. Soc.*, **2023**, *145*, 19, 10584–10594.

(2) "Photoswitchable Rhodamine-Based Multi-analyte Sensors for Metal Ions Detection" Anjali Srivastava, Surbhi Grewal, Sapna Singh, Rajani, Sugumar Venkataramani* *ChemPhotoChem.*, **2023**, Just accepted.

(3) "Does Nitrogen Lone Pair Lead to Two Centered - Three Electrons (2c-3e) Interactions in Pyridyl Radical Isomers?" Chitranjan Sah, Lilit Jacob, Mayank Saraswat, Sugumar Venkataramani* *J. Phys. Chem. A.*, **2017**, *121* (19), 3781-3791.



Group Members: (Front row): Shubham, Keerthi, Ramanpreet, Rajani, Gayathri, Anjali, Adithya, (Middle row): Arunima, Dr. Archana, Sugumar, Piyush, Shabana, Deepak, (Back row): Debapriya, Sapna, Ashish, Sachindeev, Himanshu.

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Associate Professor
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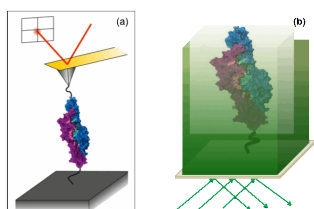
Single-Molecule Biophysics

Ph.D – 2003-09/Indian Institute of Science, Bangalore, India.

Postdoc – 2009-13/Iowa State University, USA.

Research Interests

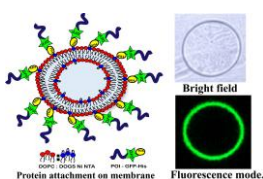
Mechanotransduction in hearing at the single molecule level



In hearing, sound waves first generate oscillations in the inner-ear fluid, which thus deflect inner-ear hair-cells and stereocilia. The stereocilia are linked together by a pair of proteins at their tips. Upon deflection, these interacting proteins at tip-links are elastically stretched, which leads to the opening of ion-channels in stereocilia. Open channels can now allow ions to move-in and change the polarity of the cells. Nerve cells attached to hair-cells thereafter sense this electrical change that is conveyed to the brain. The brain interprets this as sound.

Membrane biophysics

Using Giant unilamellar vesicles (GUV), we monitor the dynamics of enzymatic reactions and their effect on GUVs.



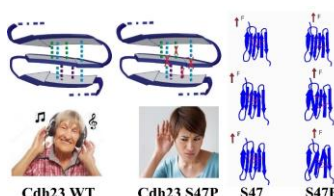
Cancer biophysics

The potential of mechanical forces in carcinoma growth is poorly understood. Currently we are exploring the role of

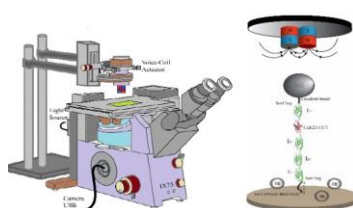
extracellular matrix proteins mediated tumour stiffness in regulating aggressiveness of glioblastoma. We employed Magnetic tweezer, rheology and atomic force microscopy, and combined cell culture studies.

Study of the hearing loss disease models

Cadherin-23 and Protocadherin-15, two tip-link proteins that actively participates in the mechanotransduction of hearing. They receive force pulses of various intensities and frequencies during the lifetime of a host. Notably, cadherin-23 protein is also one of the loci for multifactorial age-induced and noise-induced hearing loss. This implicates that the temporal loss of protein viscoelasticity with aging will cause the loss of sensory abilities.



Instrument development



Ultra-sensitive (5 nm noise) home-built magnetic tweezers provides high temporal resolution (3.5 kHz) to perform single molecule force spectroscopy at physiologically relevant force (4-200 pN) regime.

Funding

DBT-Wellcome Trust Intermediate Fellowship (Awarded, 2015-2021)
 DST Fund (Awarded, 2020-23)

Selected Publications

- (1) Kaur V, Garg S, Rakshit S. Instantaneous splicing and excision of inteins to synthesize polyproteins on a substrate with tunable linkers. *Soft Matter*. 2022 Jan 19;18(3):602-608. doi: 10.1039/d1sm01469b.
- (2) Redefining the Structure of Tip Links in Hair Cells Veerpal Kaur, Sanat K. Ghosh, Tripta Bhatia, and Sabyasachi Rakshit *Biochemistry* DOI:10.1021/acs.biochem.3c00161
- (3) Arora, N., Hazra, J.P. & Rakshit, S. Anisotropy in mechanical unfolding of protein upon partner-assisted pulling and handle-assisted pulling. *Commun Biol* 4, 925 (2021). <https://doi.org/10.1038/s42003-021-02445-y>
- (4) Tip-links serve as force-pass filter to fulfil the role of gating-springs Nisha Arora, Jagadish P. Hazra, Sandip Roy, Gaurav K. Bhati, Sarika Gupta, Abhishek Chaudhuri, Amin Sagar, Sabyasachi Rakshit doi: <https://doi.org/10.1101/2022.08.10.503460>
- (5) Heterogeneity in conformational state space enhances the force-tolerance of mechanosensory proteins Pritam Saha, Vishavdeep Vashisht, Ojas Singh et al. 23 March 2023, <https://doi.org/10.21203/rs.3.rs-2677234/v1>

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Ultrafast Spectroscopy and Optical Trapping: Theory and Experiment

Profile

Ph.D – 2005-10/Indian Institute of Technology Kanpur/Prof. D. Goswami

Postdoc– 2010-14/Lawrence Berkeley National Laboratory/University of California Berkeley/Prof. G. R. Fleming

Research Interests

The central theme of research in the “Condensed Phase Dynamics” group at IISER Mohali led by Dr De is to explore, through a combination of experiments and theories, a wide range of problems in chemistry, biophysics, and condensed matter physics. More specifically, the main focus of the group is to investigate energy and charge (electron/hole or proton) transfer dynamics, covering a wide range of timescales (few tens of femtoseconds to few tens of nanoseconds), within a variety of systems (i.e., molecular aggregates, photovoltaic systems and fluorescent proteins) and the effect of the local environment (i.e., solvation and nanoscale confinement) on

To achieve this, the group has developed some cutting-edge spectroscopic techniques (i.e., sub-20 fs broadband pump-probe spectroscopy, two-dimensional electronic spectroscopy, pump-dump-probe spectroscopy, broadband (time-resolved) impulsive stimulated Raman spectroscopy and multimodal optical trapping integrated with holographic beam shaping) each of which is first of its kind developed in India.

For more details, please visit our research group website:

<https://dynamicsiiserm.wixsite.com/webpage>

Funding:

IISER Mohali (Start-up grant)

SERB, DST Early Career Research Award (ECR/2016/000467)

SERB, DST Early Career Research Award (CRG/2021/003981)

First experiment on optical and thermal nonlinearities in laser trapping

(3) “Ultrafast excited state dynamics of tricarbocyanine dyes probed by two-dimensional electronic spectroscopy: Polar solvation vs photoisomerization” Y. Silori, P. Seliya and A. K. De, *J. Phys. Chem. B*, **2020**, 124, 6825.

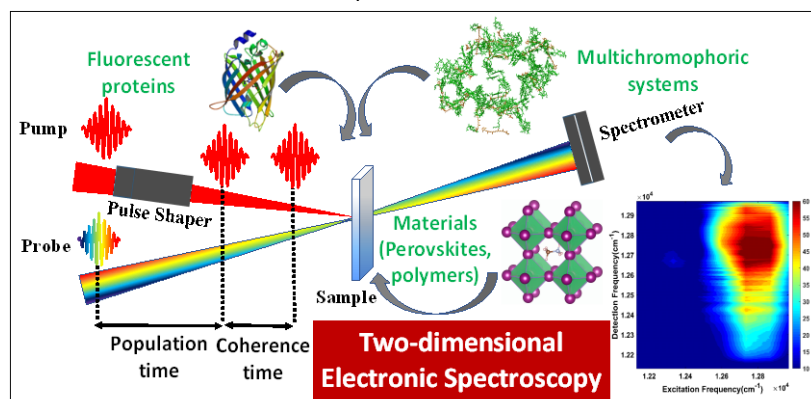
First experiment using two-dimensional electronic spectroscopy.

(4) “A revisit on impulsive stimulated Raman spectroscopy: Importance of spectral dispersion of chirped broadband probe” S. Dhamija, G. Bhutani, A. Jayachandran and A. K. De, *J. Phys. Chem. A*, **2022**, 126, 1019.

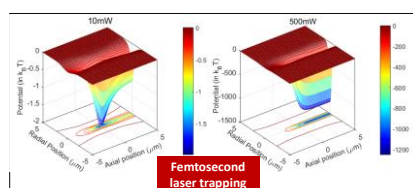
First experiment on broadband impulsive stimulated Raman spectroscopy.

(5) “Elucidating structure-property relationship and ultrafast exciton/charge-carrier dynamics of layered $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ double-perovskite microcrystals” S. Mishra, S. Sapru, S. N. Upadhyay, A. Singh, S. Pakhira and A. K. De, *J. Phys. Chem. C*, **2023**, 127, 1811.

(6) “Unveiling Role of Hidden Isomers in Large Stokes Shift in mKeima: Harnessing pH-Sensitive Dual-Emission in Bio-imaging” G. Bhutani, P. Verma, A. Jayachandran, S. Pal, K. Chattopadhyay and A. K. De, *J. Phys. Chem. B*, **2022**, 12, 3197.



it. The group also pioneered in deciphering the role of optical and thermal nonlinearities in laser trapping under femtosecond pulsed excitation.



Selected Publications

(1) “Theoretical investigation on nonlinear optical effects in laser trapping of dielectric nanoparticles with ultrafast pulsed excitation” A. Devi and A. K. De, *Optics Express*, **2016**, 24, 21485.

First conceptualization of nonlinear optical trapping:

(2) “Dynamics of a dielectric microsphere inside a nonlinear laser trap,” A. Devi, S. Yadav and A. K. De, *Appl. Phys. Lett.*, **2020**, 117, 161102.



Front Row (L to R): Shaina, Garima, Sakshi, Samita, Yogita, Umang and Anita
 Back Row (L to R): Arindam, Subho, AKDe, Subhash, Dharam and Sumit

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Nanomaterials and Renewable Energy

Profile:

Ph.D – 1999-2006/Indian Institute of Science

Postdoc– 2006-08/National Institute for Materials Science, Tsukuba, Japan

ICYS-Independent researcher-2008-11

Ramanujan Fellow – 2011-14, JNCASR, Bangalore

Research Interests:

Our research work is focused on developing functional nanomaterials and their applications in energy harvesting and environmental remediation. It requires involvement in photocatalysis, electrocatalysis, in-situ investigations of reaction kinetics, excitons dynamics, surface characterization techniques, and high-resolution structural analysis using electron and atomic force microscope.

Nanomaterials for energy harvesting and environmental remediation:

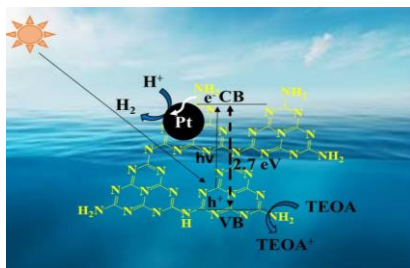
Nanomaterials with excellent activity, high selectivity, and stability are required and their properties can be tuned by tailoring the size, shape, and morphology. In the *Nanomaterials and Renewable Energy Laboratory*, we plan to develop various functional nano and nano-hetero-materials with specific shapes, sizes and morphologies as heterogeneous catalysts and then evaluate their efficiency toward **(a)** photocatalytic and piezocatalytic water splitting and hydrogen energy harvesting, **(b)** oxygen reduction or fuel oxidation reaction **(c)** oxygen harvesting using carbon quantum dots.

Electrocatalysis:

We design and synthesize new generation catalysts for boosting electrocatalytic oxygen evolution and reduction, a key step in promising sustainable energy conversion technologies such as fuel-cell and energy storage batteries.

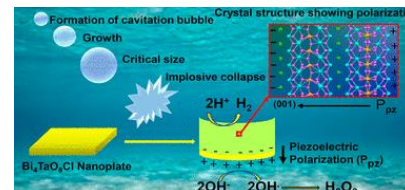
Photocatalytic water splitting:

The generation of green hydrogen from photocatalytic water splitting has gained tremendous research interest leading to the development of a large number of photoactive materials. We also investigate the metal-free graphitic carbon nitride (*g*-C₃N₄) nanostructures as photocatalytic materials.



Piezocatalytic water splitting:

Piezocatalysis, a newly developed technology has demonstrated tremendous promise for hydrogen production that can overcome demerits of electrocatalytic and photocatalytic approaches. The purpose of the research is to develop a new class of layered perovskite oxyhalide materials with highly efficient piezocatalytic hydrogen production efficiency even in the absence of any cocatalyst and scavenger, besides using them for H₂O₂ generation and other fine chemicals as well.



Selected Publications:

- (1) "Covalently interconnected layers in *g*-C₃N₄: Toward high mechanical stability, catalytic efficiency and sustainability.", Roy, R. S., Mondal, S., Mishra, S., Banoo, M., Sahoo, L., Kumar, A., Vinod, C. P., De, A. K. and Gautam, U. K. *Applied Catalysis B: Environmental*, 2023, 322, p.122069.
- (2) "Light-induced hypoxia in carbon quantum dots and ultrahigh photocatalytic efficiency.", Mondal, S., Das, S. R., Sahoo, L., Dutta, S., & Gautam, U. K.*, *J. Am. Chem. Soc.*, 2022, 144, 2580-2589.
- (3) "Bi₄Ta_{0.8}Cl as a New Class of Layered Perovskite Oxyhalide Materials for Piezopotential Driven Efficient Seawater Splitting.", Banoo, M., Roy, R. S., Bhakar, M., Kaur, J., Jaiswal, A., Sheet, G., & Gautam, U. K.*, *Nano Letters*, 2022, 22, 8867-8874.
- (4) "Ultrathin twisty PdNi alloy nanowires as highly active ORR electrocatalysts exhibiting morphology-induced durability over 200 K cycles." Sahoo, L., Garg, R., Kaur, K., Vinod, C. P., & Gautam, U. K.*, *Nano Letters*, 22, 2022, 246-254.

Group Members:

(From left to right) (Back) Raj, Ankit, Arjun, Komal, Jaya, Dr. Abhishek, Supriya, Vaibhav, (Middle) Riya, Dr. Ujjal, Maqsuma, (Front) Sahil, Aniket, Dr. Bramhaiah, Mukul. (Inset – Top- Kaustubh, Below- Mohit)

Balanarayan P
Associate Professor
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Tel: +91 8968216347



Theoretical and Computational Chemistry

Profile:

Ph.D – 2008/University of Pune, Pune,
Supervisor: Professor Shridhar R. Gadre

Postdoc–2009-2013/Technion, Haifa,
Israel, Mentor: Professor Nimrod
Moiseyev

Research Interests:

Our interests lie in theoretical and computational chemistry. The focus of this group is on electronic structure, and properties of atoms and molecules. Currently we are involved in the electronic structure of atoms and molecules in high intensity and high frequency oscillating fields.

Development of simulation methodologies: For understanding the behaviour of atoms and molecules in strong laser fields particularly for Attosecond electronic dynamics within the strong field, beyond-perturbation theory regime, novel methodologies need to be developed and implemented. Our group does this together with the coding validation and implementation of the methods into our own in-house software packages named ABDYN, ABELDYN and ABELDYN-PROP.

Atoms and Molecules in external fields: The properties of atoms and molecules in strong time-varying LASER fields which modifies their behaviour completely is a theme of our research.



Research Group: Quantum mechanics group at DCS, Aman Kumar Sharma (BS-MS student 2023), Ph. D. Students: Nitin Kumar Singh, Prateek Ahuja, Aman Gupta, Taseng Mancheykuhn, Kirti, Alkit Gugalia and Harwinder Kaur.

Debashis Adhikari

Associate Professor

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Synthetic Inorganic, Organometallic, Catalysis

Profile:

Ph.D.–2004-2009/Indiana University,
Bloomington, IN, USA /Daniel J. Mindiola

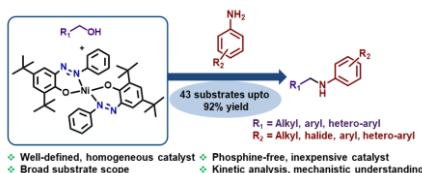
Postdoc–2010-2012/Northwestern
University, Evanston, IL, USA /Sonbinh T.
Nguyen

Professional experience–2012-
2015/Lecturer/ Indiana University,
Bloomington, IN, USA

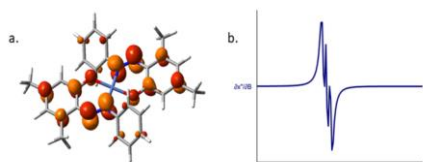
Research Interests:

1. Redox-active ligand-based metal complexes for catalysis and small molecule activation

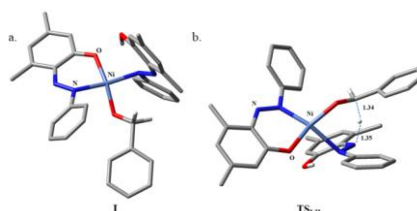
We recently reported a well-defined and bench-stable azo-phenolate ligand coordinated nickel catalyst which can efficiently execute N-alkylation of a variety of anilines by alcohol. We demonstrated that the redox-active azo ligand can store hydrogen generated during alcohol oxidation and redelivered the same to an *in situ* generated imine bond to result N-alkylation of amines. The reaction has wide scope and a large array of alcohols can directly couple to a variety of anilines. Mechanistic studies including deuterium-labelling to the substrate establishes borrowing hydrogen method from alcohols and pinpoints the crucial role of the redox active azo moiety present on the ligand backbone. Isolation of the ketyl intermediate in its trapped form with a radical quencher, higher k_H/k_D for the alcohol oxidation step suggest altogether a hydrogen atom transfer (HAT) to the reduced azo backbone to pave alcohol oxidation as opposed to conventional metal-ligand bifunctional mechanism.



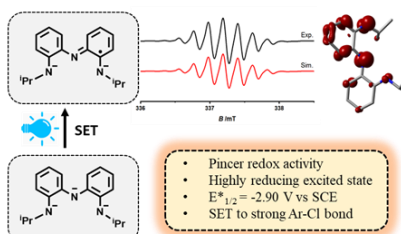
Shown here the low-lying LUMO of the complex which is azo-based and the reduction takes place mostly on that part of the ligand. Further characterization by EPR reveals that nitrogen-centric nature of the radical.



A computational probaton (DFT) further provided convincing proof for the HAT step. Shown here is an important intermediate along the reaction pathway as well as the transition state for HAT. This example showcases the tandem reactivity of nickel with a redox active ligand.



2. Photoredox chemistry



Our research motive is to find out inexpensive organic molecules which can be easily excited upon irradiation by visible light. Upon excitation these molecules often perform single electron transfer (SET) or hydrogen atom transfer (HAT) en route to valuable synthetic transformations. Such organic motifs or their anions are usually electron rich, so that they can elicit strong reductive behavior during breaking a strong C-X type bond. The resulting aryl or alkyl radicals can either lead to cross coupling reactions or an array of radical-mediated cyclization reactions. We also study the photophysical properties of the molecules at their excited states.

Shown here is a “NNN”-pincer motif that without any metal can perform strong reductive chemistry under visible light initiation.

Selected Publications:

- 1) Unexplored facet of pincer ligand: Super-reductant behavior applied to transition-metal-free catalysis. V. Singh; R. Singh; A. S. Hazari; D. Adhikari. *JACS Au*, 2023, 3, 1213-1220.
- 2) Ligand-Based Redox: Catalytic Applications and Mechanistic Aspects. K. Singh; A. Kundu; D. Adhikari. *ACS Catal.* 2022, 12, 13075–13107.
- 3) Unlocking the photo-dehydrogenation ability of naphthalene monoimide towards the synthesis of quinazolinones. S. Halder; S. Mandal; A. Biswas; D. Adhikari. *Green Chem.*, 2023, 25, 2840-2845.
- 4) Ligand-redox assisted nickel catalysis toward stereoselective synthesis of (n+1)-membered cycloalkanes from 1,n-diols with methyl ketones. A. K. Bains; A. Kundu; D. Maiti; D. Adhikari. *Chem. Sci.*, 2021, 12, 14217-14223.
- 5) Borrowing Hydrogen-Mediated N-Alkylation Reactions by a Well-Defined Homogeneous Nickel Catalyst. A.K. Bains; A. Kundu; S. Yadav; D. Adhikari. *ACS Catal.* 2019, 9, 9051-9059.



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Materials Chemistry

Profile:

PhD – 1998/*Indian Institute of Science, Bangalore*; **Thesis:** Fine Ceramic Pigments: Combustion Synthesis and Properties; **Supervisor:** Professor K.C. Patil;

Postdoc: - 1999– 2002/*Max-Planck Institute Fur Festkorperforschung, Stuttgart, Germany/Professor Arndt Simon and Dr. Peter Adler*;

Postdoc: - 2002– 2003; *Institut des Matériaux Jean Rouxel, Nantes, France*; / **Dr. Yves Piffard**;

Postdoc: - 2005– 2007; *University of Wisconsin, Milwaukee, USA*/ Professor Prasenjit Guptasarma

Professional Experience: Research Technician, 2007; *Angstrom Power Inc., Vancouver, BC Canada*

Research Interests:

Biodiesel, Green Chemistry & Undergraduate Chemistry Laboratory

(a) In the area of biodiesel, I am trying to develop cost effective techniques for obtaining transparent calcium impurity-free biodiesel in high yields from reusable calcium oxide based heterogeneous basic catalysts.

(b) In the area of Green Chemistry, I am trying to develop cost effective techniques for recovering/regenerating industrially important chemicals by recycling used alkaline dry-cell batteries. In another project, I am trying to develop and implement remediation techniques for handling large quantities of mixed waste chemicals generated in the research laboratory.

(c) Since IISER Mohali is also an educational center, my research efforts are mainly focused on issues pertaining

to undergraduate Chemistry teaching laboratory. Along with teaching laboratory staff and students, I try to:

1. Design, develop and improvise upon common tools and implements for undergraduate Chemistry laboratory which students with disabilities can use. The commercially available tools in most teaching laboratories are suitable for use only by able-bodied students.

2. Design and develop gadgets for undergraduate Chemistry laboratory which will be cheaper than the ones available commercially. Cheaper alternatives will enable more students in any undergraduate Chemistry laboratory to have access to gadgets and consequently gaining of more hands-on experience.

3. Design and develop techniques which will enable the undergraduate Chemistry laboratory to save on fuels like costly gas used for reactions involving heating operation. Typically a big batch of undergraduate students in a Chemistry laboratory will involve expending lot of gas.

4. Improvise upon existing labcoat features in order to make it more user-friendly.

5. Develop techniques which will help in minimizing maintenance efforts required for the upkeep of expensive gadgets.

6. Experiment with remediation techniques based on Fenton's process and develop management methodologies which could in near future enable big undergraduate Chemistry laboratories to implement some of these techniques and methods for taking care of the huge mixed chemical wastes that gets generated in a laboratory session comprising of a big batch of students. Presently storing and disposal of such huge mixed waste chemical waste is a big challenge. If the problem is not addressed, it could have an adverse impact on the smooth functioning of the undergraduate Chemistry laboratory.

7. Search for appropriate alternative green chemical reactions from various

sources which are less tedious and involve less hazardous chemicals for possible introduction with some improvisation to undergraduate Chemistry laboratory to circumvent generation of huge toxic waste.

8. Develop innovative laboratory notebook time saving documentation and appraisal techniques helpful for both the students and the instructors.

9. Develop simple information management system for students to handle and process wealth of data they accumulate and thereby mitigate the syndrome of information overload.

10. Further develop and improve my laboratory relevant pedagogical skills to present Chemistry subject in an innovative manner that will encourage more students to opt for Chemistry as a career.

In my endeavors, I have been successful to some extent in developing: 1. Unique semi-automatic stopcock-free burette filler which is affordable and can be operated by a wheelchair bound student. Application filed for obtaining an international patent. 2. Semi-automatic pipette filler for which an international patent has recently been granted. 3. Portable, palm size, light weight, energy efficient affordable magnetic stirrer with AC/DC power supply in collaboration with Physics teaching lab



Publications:

(1) "A semi-automatic pipette filler instrument and a modified pipette"; International Patent Number: WO 2015/092777A2 published on 25th June 2015

(2) "A new visual test for p-quinone and its relevance to the biodiesel industry", Samrat Ghosh, Shilpa Setia, Sumyra Sidiq and Santanu Kumar Pal *Analytical Methods*, **2012**, 4, 3542.

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Structural Chemistry and Crystallography

Profile:

Ph.D – 1999-2004/Indian Institute of Science, Bangalore, India/Prof. T. N. Guru Row

Postdoc – 2004-07/University of Liverpool, Liverpool, United Kingdom /Dr. Neil Winterton

Professional experience – 2007-09/Birla Institute of Technology and Science, Pilani, India; 2009-to date Indian Institute of Science Education and Research, Mohali

Research Interests:

Synthesis, Characterization and Solid State Chemistry of Small Organic Molecules, experimental and theoretical charge density analysis

Small organic molecules containing one or more fluorine atom are of structural importance due to their highly influential role in crystal packing and in altering the physical properties of the molecule. Fluorinated drugs and pharmaceutical are of utmost importance compared to their non-fluorinated analogues. Therefore, the structure directing activity of organic fluorine is studied using X-ray diffraction technique. The intermolecular interactions are best analyzed using experimental and theoretical charge density analyses, which is one of the major research activities of this group.

Metal-organic Frameworks

Metal-organic frameworks (MOFs) are important class of compounds for their application in gas absorption, drug delivery, gas or ion sensing capabilities etc. 3D organic ligands with various –COOH based linkers are being used for the generation of MOFs in our laboratory. Synthesis, characterization and structural studies on MOFs are another interest of our laboratory.

Pharmaceutical Co-crystallization and their Applications:

A number of known drugs suffer from various formulation difficulties related to their solubility, dissolution rate and thermal stability. We intend to develop novel drug composites to achieve better solubility and dissolution rates and higher thermal and storage stability of the well-known drugs through salt formation of by co-crystallization. We have been successful in generating a number of new novel formulations with better physico-chemical properties for better bio-availability of a variety of antibacterial and antifungal agents through our studies.

Experimental and Theoretical Study of Weak Intermolecular Forces Involving Organic Fluorine:

Weak interactions in the solid state are also studied using the knowledge from structural analysis in ab-initio calculations using Gaussian16 to quantify the strength of various weak interactions involving organic fluorine. Photophysical properties like cis-trans isomerization, possible dimerization of various functionalized imines and azobenzenes are also studied in our laboratory.



Current Lab Members

From Left: Sunanda, Vandana, Vierandra, Bhavna and Sakshi

In situ crystallization of low melting solids, liquids and gases and their mixtures

Crystal structures of liquids or gases are determined by *in-situ* crystallization technique. LASER assisted Optical Heating and Crystallization Device is used to grow crystals of low melting solids for their structure determination.

Selected Publications:

- (1) "Investigation of C-F...F-C Interactions Using Experimental and Theoretical Charge Density Analyses", Singla, L., Kumar, A., Robertson, C. M., Munshi, P and Choudhury, A. R. *Cryst. Growth Des.* **2023**, 23(2), 853-861.
- (2) "Structural and Computational Analysis of Organic Fluorine-Mediated Interactions in Controlling the Crystal Packing of Tetrafluorinated Secondary Amides in the Presence of Weak C-H...O=C Hydrogen Bond", *Cryst. Growth Des.* **2022**, 22(3), 1604-1622
- (3) "Understanding of the Kinetic Stability of cis- Isomer of Azobenzenes through Kinetic and Computational Studies". Das, D., Yadav, M. K., Singla, L., Kumar, A., Karanam, M., Dev, S., Choudhury, A. R. *Chem. Select.* **2020**, 5(44), 13957-13962.
- (4) "Insights into the C-H/F-C hydrogen bond by Cambridge Structural Database analyses and computational studies", Dev, S.; Maheshwari, S.; Choudhury, A. R. *RSC Adv.*, **2015**, 5, 26932.
- (5) "A comprehensive understanding of the synthons involving C-H...F-C hydrogen bond(s) from structural and computational analyses". Kaur, G.; Choudhury, A. R. *CrystEngComm*, **2015**, 17, 2949.
- (6) "In situ co-crystallization of cresols with aniline and fluoroanilines: subtle interplay of strong and weak hydrogen bonds". Choudhury, A. R.; Yufit, D. S.; Howard, J. A. K. *Z. Kristallogr.* **2014**, 229, 625.

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Theoretical and Computational Quantum Chemistry

Profile:

PhD – 1998 – 2004/ NCL, Pune, India / Prof. Sourav Pal

Postdoc: - 2004-06 / University of Waterloo / Prof. Marcel Nooijen

Postdoc: - 2007-2010 / University of Stuttgart, Germany / Prof. H. -J. Werner

Research Interests:

Development and Applications of Multi-reference electron-correlation methods for open-shell molecules:

In the past, we have been involved in development of a variant of multi-reference method using internally contracted configuration functions. Its efficiency and applicability for medium-size inorganic open-shell molecules has been established. Current focus in the group is to develop a multi-reference method for simultaneous treatment of several excited states and a multi-reference coupled-cluster method based on density matrix cumulants. Apart from this, we have also been involved in a few collaborative works on coupled-cluster methods [1] as well as the construction of accurate potential energy surfaces for nuclear quantum dynamics studies [2].

Multiply Ionized states of small molecules:

Earlier, we have carried out a study of charge symmetric dissociation of dications of N₂ and CO molecule by computing potential energy curves for several states contributing to observed kinetic energy release pattern in electron impact ionization experiments. Recently, we have applied a new procedure to compute high-lying states of molecular nitrogen with one or more core and valence holes [3].

Non-adiabatic couplings and dynamics using coupled-cluster wave-functions:

We have found a novel approach for theory and computations of non-adiabatic couplings using coupled-cluster wave-functions. Some elements of the approach have been explored in detail for diagonal Born-Oppenheimer correction [4]. To generalize this approach to possibly treat nuclear quantum dynamics of multiple excited states using coupled-cluster methods is currently under exploration.

$$-\frac{\langle\Phi|\nabla^2|\Phi\rangle}{2\langle\Phi|\Phi\rangle} = -\frac{1}{2}\left(\nabla + \frac{\langle\Phi|\nabla\Phi\rangle}{\langle\Phi|\Phi\rangle}\right) \cdot \frac{\langle\Phi|\nabla\Phi\rangle}{\langle\Phi|\Phi\rangle} + \sum \frac{\langle\Phi|\nabla X\rangle \cdot \langle\nabla\tilde{X}|\Phi\rangle}{2\langle\Phi|\Phi\rangle}$$

$$\mathcal{F}_{\beta\alpha}^{\text{CI}} = \frac{1}{\langle\Phi|\Phi\rangle} \left(\sum \langle\Phi|\partial_\beta X\rangle \langle\partial_\alpha X|\Phi\rangle - \langle\Phi|\partial_\alpha X\rangle \langle\partial_\beta X|\Phi\rangle \right) = 0$$

$$\mathcal{F}_{\beta\alpha}^{\text{CC}} = \frac{1}{\langle\Phi|\Phi\rangle} \left(\sum \langle\tilde{\Phi}|\partial_\beta X\rangle \langle\partial_\alpha \tilde{X}|\Phi\rangle - \langle\tilde{\Phi}|\partial_\alpha X\rangle \langle\partial_\beta \tilde{X}|\Phi\rangle \right) \neq 0$$

Magnetic spin-state energy gaps in organic tri-radicals:

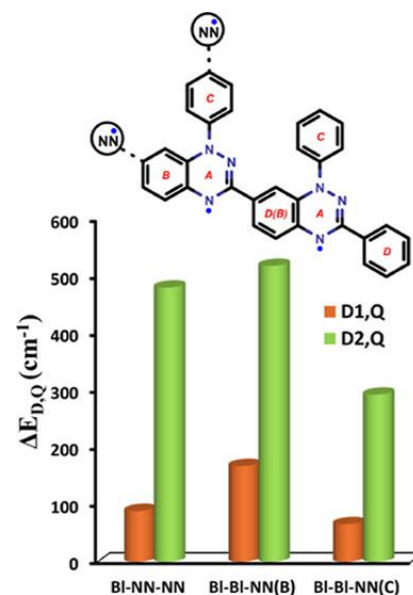
Recently, in collaborative work, we have computationally studied the quartet-doublet energy gaps of several organic tri-radicals based on Blatter's radical [5]. We have systematically applied high-level multi-reference methods to compute all the states of spin-multiplet arising from tri-radical character and established their reliability in comparison to excited states. Further studies on tetra-radical possibilities are being explored in collaboration. A new theoretical procedure to compute magnetic exchange couplings for multi-center radicals is also under development.

Aromaticity Indices:

A student is exploring in a master's thesis on understanding how aromatic indices capture this important notion in chemistry.

Recent Publications:

1. J. Black, A. Waigum, R. G. Adam, K. R. Shamasundar, A. Kohn, *J. Chem. Phys.* **158**, p134801 (2023)
2. B. Mukherjee, K. Naskar, S. Mukherjee, Satyam Ravi, K. R. Shamasundar, D. Mukhopadhyay, S. Adhikari, *J. Chem. Phys.* **153**, p174301 (2020)
3. D. Bhattacharya, K. R. Shamasundar, A. Emmanouilidou, *J. Phys. Chem. A* **125**, p7778 (2021)
4. K. R. Shamasundar, *Mol. Phys.* **116**, 1483 (2018)
5. R. Khurana, A. Bajaj, K. R. Shamasundar, E. Ali, *J. Phys. Chem. A*, **127**, p7802 (2023)



(Former Group Members From left: Satyam, Sham and Jitendra)

Sanchita Sengupta

Assistant Professor

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Functional Organic Materials

Profile:

Ph. D – Dec 2011/University of Würzburg, Germany /Prof. Dr. Frank Würthner.

Postdoc–2012-Jun2013/ Delft University of Technology, The Netherlands /Prof. Ferdinand C. Grozema, Prof. Wolter Jager.

Professional experience – Aug 2013-Apr 2017/Indian Institute of Science (IISc) Bangalore/DST INSPIRE faculty fellow.

Research Interests:

1. Functional Materials based on BODIPY and Squaraine Dyes towards Optoelectronic Applications and Photocatalysis: Donor-acceptor (D-A) light harvesting systems (in configurations such as D-A-D, A-D-A, D-A-A etc.) for efficient photoinduced electron transfer (PET) will be designed and investigated. Major emphasis will be given on their synthesis, photophysics, charge carrier mobilities and electronic properties in order to assess their suitability in photoconduction for eventual integration in organic photovoltaic (OPV) devices. Such synthesized D-A conjugates are also being utilized as photocatalysts in organic transformations in our group.

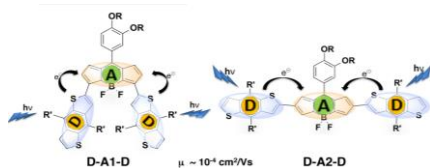


Fig 1. Schematic representation of regioisomeric D-A-D systems with efficient PET and charge carrier mobilities.

2. Multichromophoric Light Harvesting Antenna Systems for Efficient Energy Transfer: Covalently connected multichromophoric light-harvesting (LH) systems (based on perylene diimide, aza-BODIPY, naphthalimide and a few other classes of molecules with complementary absorption) with the aim of achieving efficient Förster resonance energy transfer

(FRET) are being designed in our group. Design strategies involve covalent synthesis in a manner such that chromophores can be positioned with favorable orientations for FRET. Such FRET based LH antennae have also been utilized as multifunctional sensors that are responsive to multiple stimuli such as temperature, pH, addition of metal ions, variation in redox potentials. They have also been utilized as reversible fluorescent inks.

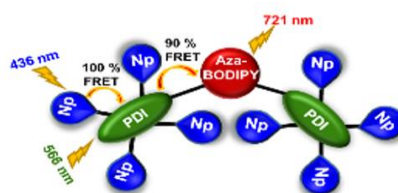


Fig 2. Representation of multichromophoric FRET LH system designed in our group.

3. Twisted Donor-Acceptor Molecular Architecture: Covalently connected conformationally restricted new D-A systems with variable spacer unit(s) will be designed for twisted intramolecular charge transfer (TICT) or thermally activated delayed fluorescence (TADF). Fundamental structure-property relationships of these materials will be deduced through structural and optical characterization. Eventually, the application of some of the screened materials in energy transfer mediated or electron transfer mediated photocatalysis will be explored.

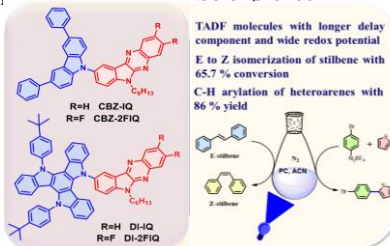


Fig 3. Diindolocarbazole and phenyl carbazole based TADF conjugates for energy transfer- and electron transfer-mediated photocatalysis.

Selected Publications:

(1)“Functionalized Benzothiadiazole Non-fused A-D-A'-D-A Small Molecules for Effective Electron Mobilities and Metal-free Photocatalysis” N. P. Tripathi, V. Gupta, T. Tarun, U. K. Pandey and S. Sengupta* *Chem. Eur. J.* **2023**, e202203951(1–8).

(2)“Metal-free FRET Macrocycles of Perylenediimide and Aza-BODIPY for Multifunctional Sensing.” K. Rani and S. Sengupta* *Chem. Commun.*, **2023**, 59, 1042–1045.

(3)“Unravelling the Excited State Dynamics of Monofunctionalized Mono- and Di-styryl BODIPY and Perylenediimide Dyads.” K. Rani, S. Chawla, V. Kumari, A. K. De* and S. Sengupta* *J. Mater. Chem. C* **2022**,10, 10551–10561.

(4)“Multi-stimuli Programmable FRETbased RGB Absorbing Antennae Towards Ratiometric Temperature, pH and Multiple Metal Ion Sensing.” K. Rani and S. Sengupta* *Chem. Sci.*, **2021**, 12, 15533–15542.

(5)“Regioisomeric BODIPY-Benzodithiophene Dyads and Triads with Tunable RedEmission as Ratiometric Temperature and Viscosity Sensors.” Aswathy P. R., S. Sharma, N. P. Tripathi and S. Sengupta* *Chem.-Eur. J.* **2019**, 25, 14870–14880. (Hot Paper).

Funding (after 2019): MoE STARS grant (2023-26), SERB-POWER grant (2022-25).



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Molecular Strong Coupling Lab

Profile:

Ph.D – 2012/National Institute for Interdisciplinary Science and Technology -CSIR, Thiruvananthapuram, India.
 Supervisor's name: K. George Thomas

Postdoc – 2012-17/University of Strasbourg, Strasbourg, France
 Mentor's name: Thomas W. Ebbesen

Research Interests:

Strong Light-Matter Interactions
Active Plasmonics
Photophysics and Photonics

Our group activities are highly interdisciplinary in nature. We study strong interactions between light (photon) and molecules by placing them in the confined electromagnetic field of a cavity or a plasmonic nanostructure. A molecule exchange energy between the cavity and the molecular state through Rabi oscillations (resonance interaction) creating two new eigen states called as polaritonic states (**Figure 1**). At ON resonance conditions polaritonic states are half-molecule and half-photon like, they show very interesting chemical and physical properties.

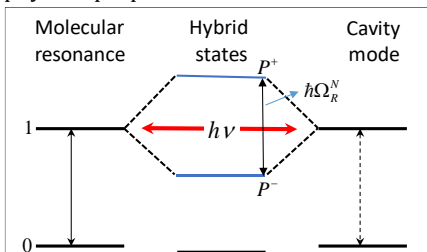


Figure 1: Light-matter hybridization of a cavity and a molecular state.

Our group is mainly focusing on two aspect of these strong interactions. They are broadly divided under the umbrella of chemistry and material science. Two of the ongoing projects are mentioned below.



From left top: Pooja, Anand, Pallavi, Kuljeet, Ben, and Jaibir.

From left bottom: Dasthaheer, Jino, Aline, Jhuma, Akhila, and Nitin (August 2023)

Project 1: Polaritonic Chemistry

Strong coupling of light to a vibrational transition should affect chemistry because it offers a simple way to modify a given chemical bond and hence their reactivity landscape. We study the kinetics and dynamics of chemical reactions in microfluidic flow cell cavities and the energy level get modified as shown in the **Figure 2**.

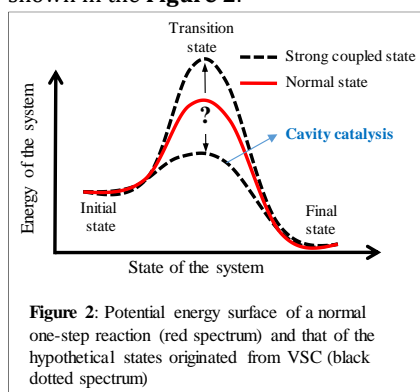


Figure 2: Potential energy surface of a normal one-step reaction (red spectrum) and that of the hypothetical states originated from VSC (black dotted spectrum)

Project 2: Polaritronics

Here, more emphasis will be given for improving the efficiency of energy and electron transport in molecular materials via the polaritonic states-new field of research coined as 'polaritronics'. Such systems will be tested in a home built electro-optical work station for measuring their charge transport and optical properties simultaneously.

Recent Publications (2023):

1. Bhatt, P.; Dutta, J.; Kaur, K.; George, J. Long-Range Energy Transfer in Strongly Coupled Donor-Acceptor Phototransistors. *Nano Lett.* **2023**, 23 (11), 5004-5011.
2. George, J.; Singh, J. Polaritonic Chemistry: Band-Selective Control of Chemical Reactions by Vibrational Strong Coupling. *ACS Catalysis* **2023**, 2631-2636.
3. Kaur, K.; Bhatt, P.; Johns, B.; George, J. Interaction of Confined Light with Optically Structured Thin Film Organic Semiconductor Devices. *arXiv preprint arXiv:2301.10421* **2023**.
4. Singh, J.; Lather, J.; George, J. Solvent Dependence on Cooperative Vibrational Strong Coupling and Cavity Catalysis. *Chemphyschem* **2023**, 24, e202300016.

Funding:

DST-SERB- EMR/2017/003455
 MoE-STARS/STARS- 1/175

Our websites:

Group: <https://jinobey.wixsite.com/msc-group>

Scholar:

<https://scholar.google.com/citations?user=fz5Nf7QAAAAJ&hl=en&oi=ao>

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Polymer Chemistry

Profile:

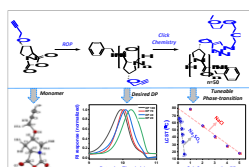
Ph.D – 2008-2012/ Indian Institute of Science Bangalore /Prof. S Ramakrishnan

Postdoc–2012-2015/ Institut Charles Sadron, Strasbourg /Prof. Jean-Francois Lutz/ 2015-2017/ Nagoya University/ Professor Eiji Yashima

Research Interests:

Our research group is multi-disciplinary in nature and situated at the interface of Organic, Physical and Material Chemistry. As a Polymer Chemistry research group, our motto is to design and synthesis of new functional polymers for targeted applications. We endeavor through development and adaptation of synthetic methodology along with extensive physical characterization to achieve our research objectives. Our major research activities are shown below.

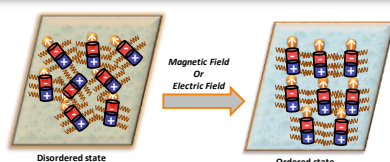
(A) Design and Synthesis of Functional Polypeptides:



Having the same backbone as proteins, synthetic peptides make interesting biomaterials. Polypeptides are often synthesized in one step using controlled ring-opening polymerization (ROP) of N-carboxyanhydride monomers (NCA), in contrast to discrete oligopeptide synthesis (SPPS). Among them we are particularly interested with polyprolines.

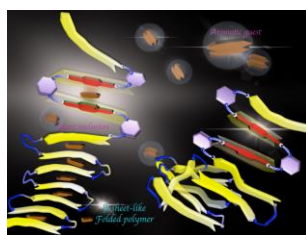
(B) Organic multiferroic materials

Magnetism and ferroelectricity are two key components for various technological applications and which are generally mutually exclusive in nature. However, it has been suggested that intimating those two effects could lead to an interesting cross-coupling phenomenon.



In this context, our approach will be to organize the electric and magnetic dipoles on a foldamer scaffold to achieve the multiferroic properties.

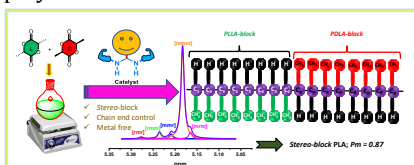
(C) Charge-transport through spatially organized π -electron rich macromolecules



It is well understood that the superior functions of the biomolecules are deeply rely on their higher order structure. In this context, we are trying to organize π -electron rich moieties by using covalent as well as non-covalent interactions to create a charge transport channel across the π -surface.

(D) Development of organocatalyst for the ROP of Lactides:

It has been shown in the past that many metal alkoxides and organometallic catalysts can promote stereoregular PLA synthesis. Despite the spectacular successes of organometallic catalysts, toxic and metal contamination caused by them paved the way for the development of organocatalysts. We were interested in developing new organocatalysts that facilitate the synthesis of stereoregular polylactides.



Left to right: Anish, Prabir, Raj, Arjun, Deepak, Subhendu, Umer, Ankita and Ankita Meena.



Selected Publications:

(1) "Comparison of Thermoresponsive Behavior between Polyproline and Periodically Grafted Polyproline toward Hofmeister Ions: An Explanation of Its Conformational Origin" A. S. Bisht, P. Maity, R. K. Roy. *Macromolecules* **2023**, 56, 3922.

(2) "Synergetic H-Bonding and C-T Interaction-Mediated Self-Assembled Structure Results in a Room-Temperature Ferroelectric Material Exhibiting Electric Field-Induced Dipole Switching and Piezo- and Pyroelectric Energy Conversion" Deepak, Z. Mallick, U. Sarkar, D. Mandal, and R. K. Roy. *Chem. Mater.* **2023**, 35, 3316.

(3) "Architectural Effect on Self-Assembly and Biorecognition of Randomly Grafted Linear and Branched Polymers at Liquid Crystal-Water Interfaces" A. Kumari, I. Pani, M. Umer Lone, A. Aggarwal, S. K. Pal, and R. K. Roy. *ACS Appl. Mater. Interfaces* **2023**, 26, 31233.

(4) "Folding of aromatic polyamides into a rare intrachain β -sheet type structure and further reinforcement of the secondary structure through host-guest interactions". S. Samanta, D. Mallick, R. K. Roy. *Polymer Chemistry* **2022**, 13, 3284.

Funding:

- 1) IISER Mohali (Start-up grant)
- 2) SERB Early career 2018

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Chemistry of Biomolecular Systems

Profile

Ph.D – 2008-13/Indian Association for the Cultivation of Science, Kolkata, India/Prof. Prasanta Kumar Das

Postdoc– 2013-17/University of Padova, Italy/Marie Curie Fellow/Prof. Leonard Prins

Postdoc– 2017-18/Pennsylvania State University, USA/ Prof. Ayusman Sen

Research Interests

Since centuries, chemistry as a subject is mainly focused on the challenges of making, purifying and studying compounds. However, for the chemists, still there remains a large void in terms of understanding and mimicking the chemistry of autonomous functioning of cell and eventually life. This led to develop a new branch of chemistry named systems chemistry where the challenges are to create a synthetic organism (de novo form of life) both for better understanding the inner functioning of biology and also to create engineered life forms. Overall, the research area will be multidisciplinary, encompassing the area of (bio)organic chemistry, colloidal chemistry, nanotechnology and flow chemistry. Our prime research activities are in the following directions –

Dynamic self-assembly: In this context it is worthy to mention that one of the

fundamental feature of life is that it operates out-of-equilibrium and it needs constant influx of energy to remain in a dynamic state. This inspires us to develop synthetic system (involving enzymes) which are chemical fuel-responsive and transient in nature.

Chemotaxis of biomolecules: Directional movement of bioorganism either toward or away from a specific chemical gradient is known as chemotaxis. Understanding this phenomenon at molecular scale is gaining importance not only for the interpretation of transport at cellular level but also towards engineering nanoscale objects. Herein, we will investigate the migratory and assembly behavior of different biomolecules.

Biocatalysis driven microscale flow in confined space: Catalytic energy can be converted to mechanical energy to drive the flow of a surrounding fluid which can be achieved by surface-bound enzymatic catalysis in microchambers.

We are also interested to investigate **biocatalysis in self-organized media** to understand the behavior of surface- and volume-confined enzymes in cellular environment.

For more details, please visit our research group website:

<https://subhabratamaiti.wixsite.com/my-site>

Selected Publications

(1) Ekta Shandilya, Subhabrata Maiti. "Self-Regulatory Micro- and Macroscale Patterning of ATP-Mediated Nanobioconjugate". *ACS Nano* **2023**, 17 (5), 5108-5120

(2) Aastha, Priyanka, Subhabrata Maiti. "Simultaneous quantification of serum albumin and gamma globulin using Zn(ii)-metallo-surfactant via a coffee ring pattern" *Chem. Commun.* **2023**, 59, 6536-6539

(3) Rishi Ram Mahato, Priyanka, Ekta Shandilya and Subhabrata Maiti. "Perpetuating enzymatically-induced spatiotemporal pH and catalytic heterogeneity of a hydrogel by nanoparticles". *Chem. Sci.*, 2022.

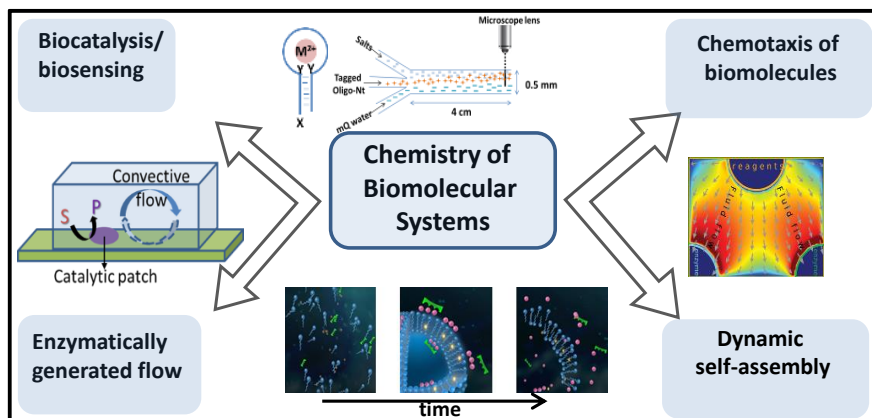
(4) Priyanka, Ekta Shandilya, Surinder K Brar, Rishi Ram Mahato, Subhabrata Maiti. "Spatiotemporal Dynamics of Self-assembled Structures in Enzymatically Induced Agonistic and Antagonistic Conditions". *Chem. Sci.*, 2022, 13, 274-282.

(5) Shikha, Ekta Shandilya, Priyanka, Subhabrata Maiti. "Directional migration propensity of calf thymus DNA in gradient of metal ions". *Chem. Commun.*, **2022**, 58, 9353-9356

(6) Rishi Ram Mahato, Ekta Shandilya, Basundhara Dasgupta, Subhabrata Maiti. "Dictating Catalytic Preference and Activity of a Nanoparticle by Modulating Its Multivalent Engagement" *ACS Catalysis*, 2021, 11, 8504-8509

Group members:

Ekta Shandilya (Thesis submitted), Akshi Deshwal (PhD degree obtained on July, 2023), Priyanka, Rishi Ram Mahato, Nandha, Shikha, Neetu, Sakshi, Reena, Paramananda Padi (Postdoc)



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Assistant Professor
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Tel: +91 9452035275



Bioinorganic and Renewable Energy

Profile:

Ph.D – 2008-2014/Indian Institute of Technology Kanpur

Postdoc– 2014-2015/CEA-Grenoble France, 2016/NPDF at IISER Kolkata

2016-2020/University of California Irvine, USA

Research Interests:

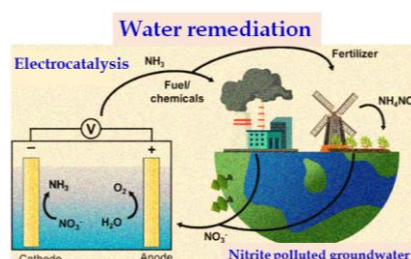
Our research interest is inspired from naturally occurring metalloenzymes, which performs unique chemical transformations with high reactivity and selectivity. We try to understand the structure-function relationship of enzymatic processes with small molecule synthetic model systems and unravel the mechanistic details. Our research is broadly focused on biomimetic small molecule activation and electrocatalysis from the perspective of environmental remediation and renewable energy.

Bioinspired Nitrite/Nitrate reduction:

Nitric Oxide (NO) plays numerous important roles in biology such as neurotransmission, blood vessel vasodilation, platelet aggregation and as antimicrobial agent. NO is produced by the reduction of nitrite in nature by Fe-containing enzymes like deoxyhemoglobin and cytochrome c oxidase (CcO) and Cu-containing enzyme copper nitrite reductase (CuNiR). The reaction carried out by CuNiR is as below $\text{Cu(I)} + \text{NO}_2^- + 2\text{H}^+ \rightarrow \text{Cu(II)} + \text{NO} + \text{H}_2\text{O}$. Beside biological importance, nitrite reduction also draws attention from environmental and health issues. Nitrogen oxyanions such as nitrate is the major nitrogen-containing toxic waste in water. This makes supply of clean drinking water challenging. In vivo nitrate reduction results in nitrite. Thus, increased nitrate concentration causes

toxicity of the nitrite which is surmised as carcinogen and causes methaemoglobinemia.

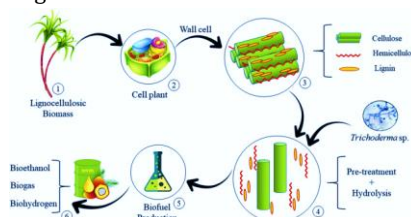
Inspired by CuNiR we develop bioinspired Cu(II) complexes and study their ability for electrocatalytic nitrite and nitrate reduction. We focus on understanding the effect of second coordination sphere in controlling the electrocatalytic nitrite reduction to NO as well as NH_3 .



Beside electrocatalytic reduction we are exploring nitrite reduction by oxygen atom transfer (OAT) and proton-coupled-electron (PCET) route as well.

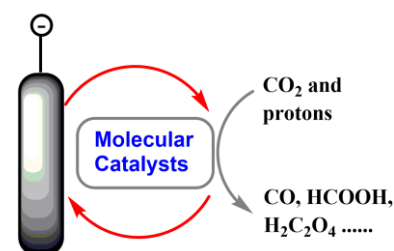
Bioinspired polysaccharides degradation: biofuels from biomass

Polysaccharide like chitin and cellulose degradation is considered as important commercial alternative for the biofuel production. Lytic polysaccharide monooxygenases (LPMOs) enzyme performs these degradations effectively. LPMOs contain mononuclear Cu(II) in the active site. Inspired by LPMOs we are developing mononuclear Cu(II) complexes for effective polysaccharide degradation.



Electrocatalytic CO₂ and proton reduction: Renewable energy

Search for earth abundant as well as economically viable renewable energy sources is one of the challenging research interests now. Keeping in mind the unprecedented levels of CO₂ at current time, a possible solution could be the recycling of CO₂ to fuels. Electrochemical reduction of CO₂ and protons offers a promising approach to produce value-added chemicals and H₂ (energy carrier)



In this context we are developing electrocatalyst for effective CO₂ reduction and H₂ evolution. We are focused on understanding mechanistic aspects and criteria for efficient and selective electrocatalysis.

Selected Publications:

(1) "Dangling Carboxylic Group That Participates in O–O Bond Formation Reaction to Promote Water Oxidation Catalyzed by a Ruthenium Complex: Experimental Evidence of an Oxide Relay Pathway", A. Kundu, S. K. Barman S. Mandal, *Inorg. Chem.*, 2022, *61*, 1426-1437.

(2) "Flavonol dioxygenation catalysed by cobalt(ii) complexes supported with 3N(COO) and 4N donor ligands: a comparative study to assess the carboxylate effects on quercetin 2,4-dioxygenase-like reactivity", N. Poddar, A. Saha, S. K. Barman, S. Mandal, *Dalton Trans*, 2023, in press.

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Molecular Magnetism and Heterogeneous Catalysis

Profile:

Ph.D. – 2012-2016/IITB-Monash Research Academy, IIT Bombay.

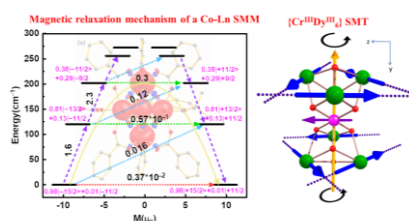
Postdoc – 1) 2017-18/Texas A&M University, USA. 2) 2019-20/Institute for Molecular Science, Japan. 3) 2020-2021/IIT Bombay, India.

JSPS Postdoctoral Fellow – 2021-22, Tokyo Metropolitan University, Japan.

Research Interests:

Our research work mainly deals with the synthesis and modeling of various molecular nanomagnets such as Single-Molecule Magnets (SMMs), Single-Molecule Toroids (SMTs), and Spin-Crossover (SCO) materials. We use SQUID magnetic instrumentation to characterize these magnetic complexes. To further understand the observed magnetic behavior of synthesized molecules, we employ both density functional theory (DFT) and *ab initio* methods using various quantum mechanics programs. We also research the metal oxide three-way catalyst to minimize the environmental impacts (CO, NO and hydrocarbons) while combusting fuels from the automobile engines.

1) SMMs: Certain metal complexes are capable of retaining their magnetization in the absence of a magnetic field which gives rise to magnetic hysteresis at a molecular level and an ability to act as magnets below their blocking temperature and these molecules are termed Single-Molecule Magnets (SMMs) or Single-Ion Magnets (SIMs). We deal with the synthesis and modeling of spin-Hamiltonian parameters in transition metals, lanthanide, and radical-bridged SMMs using both experimental and computational tools. These SMMs have intriguing potential applications in memory storage devices, spintronic devices, and Q-bits.

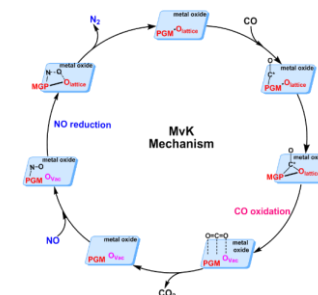


2) SMTs: We also focus on Single-Molecule Toroids (SMTs), which are defined as molecules that display a toroidal magnetic state which can potentially be used in multiferroic materials. We study the toroidal magnetism in planar rings such as {Dy₃} triangles, {Dy₄} squares, {Dy₆} hexagons, and 'double triangular' {Dy₃CrDy₃} clusters that shows the rare phenomenon of ferrotoroidal behavior.

3) SCO: The change in spin state exhibited by certain metal complexes under the application of external factors like temperature, pressure, irradiation of light, and the magnetic field is referred to as "Spin-Crossover (SCO)" or "Spin transition". We study the SCO behavior of 3d⁴ – 3d⁷ ions such Fe(II), Co(II), and Mn(II) in an octahedral ligand geometry with N₄O₂, N₃O₃ type of moderate ligands.

4) Heterogeneous Catalysts: The main areas of catalysis are focusing on minimizing the environmental impacts while combusting fuels from automobile engines. Our group is searching for the

three-way catalyst (TWC) of a car that exploits three reactions which include NO reduction, CO oxidation, and oxidation of unburnt hydrocarbons. We are adopting the computational approach to understand CO and NO adsorption and to intensively seek a suitable metal oxide surface for the investigation of the NO-CO reaction mechanism. We perform slab model calculations by spin-polarized DFT methods using the VASP program.



Selected Publications:

- (1) "Exploiting Strong {Cr^{III}-Dy^{III}} Ferromagnetic Exchange Coupling to Quench Quantum Tunneling of Magnetization in A Novel {Cr^{III}₂Dy^{III}₃} SMM", D. Chauhan, K. R. Vignesh,* A. Swain, S. K. Langley, K. S. Murray, M. Shanmugam, G. Rajaraman, **2022**, *Cryst. Growth Des.*, **23**, 197–206.
- (2) "Efficient synthetic route to heterobimetallic trinuclear complexes [Ln-Mn-Ln] and their single molecule magnetic properties" N. F. Ghazali, K. R. Vignesh, W. Phonsri, K. S. Murray, P. C. Junk, G. B. Deacon, D. R. Turner, *Dalton Trans.*, **2022**, **51**, 18502–18513.
- (3) "Slow magnetization relaxation in a rare family of triangular {Co^{III}₂Ln^{III}} clusters: the effect of diamagnetic Co^{III} ions on the Ln^{III} magnetic dynamics" A. S. Armenis, V. Vipanchi, K. N. Pantelis, L. Cunha-Silva, K. R. Vignesh, D. I. Alexandropoulos, T. C. Stamatatos, *Chem. Eur. J.*, **2023**, e202302337.



(From left): Vipanchi, Esha, Imon, Dr. Vignesh, Amit, Sriram, Joel and Manoj

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Theoretical and Computational Chemistry

Profile:

PhD – 2009-2015/Indian Institute of Science Education and Research Thiruvananthapuram

Postdoc – 2016-2018/Department of chemistry and chemical biology, Cornell University, USA

Professional experience – 2019-2020/DST Inspire Faculty, Solid State and Structural Chemistry Unit, Indian Institute of Science Bengaluru.

2021-2023/DST Inspire Faculty, Department of Chemistry, Indian Institute of Technology Palakkad

Present/Assistant Professor, Department of Chemical Sciences, Indian Institute of Science Education and Research Mohali

Research Interests:

The broader theme of our research is “chemical bonding across the periodic table”. We try to understand the factors that decide the structure, bonding, reactivity, and properties of compounds, because that knowledge will help us to tune these factors in a desirable way. We extensively use the molecular orbital theory and orbital interactions to make useful predictions, which are then confirmed by quantum chemistry calculations.

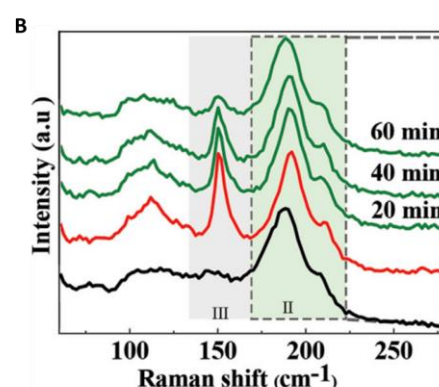
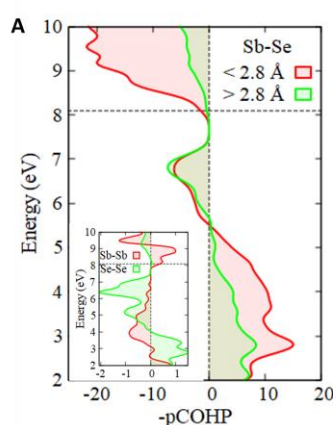
We pursue both basic and applied research. In the former, the main goal is to gain a better understanding on concepts such as Lewis acidity, hypervalency, aromaticity, multiple bonding etc. Here we try to fill the gaps in our knowledge, by providing a conceptual insight and support that by quantum chemistry calculations. We also try to translate the molecular concepts to extended solid-state structures with the intention to make material chemistry friendlier to chemists.

In the applied research, we are trying to tackle relevant technological problems such as the instability issues of the lead-iodide based perovskites which hinder their applications in commercial perovskite-based solar cells. We also try to design new materials that are potential solar absorbers and can be a good substitute for the toxic and unstable lead iodide-based perovskites.

We are also interested in semiconducting materials that exhibit the property of photoinduced phase transition and self-healing. Antimony trichalcogenides and chalcogenides are examples for such compounds. This research is aimed at understanding what structural and bonding feature is responsible for this property. Understanding this will be useful for predicting and synthesizing many such semiconducting materials, with longer life span, which is very desirable when it comes to making devices such as photovoltaic cells.

Selected Publications:

1. “On the Instability of Iodides of Heavy Main Group Atoms in their Higher Oxidation State.” C. P. Priyakumari* and Sathya S. R. R. Perumal, *Phys. Chem. Chem. Phys.* **2023**, 25, 6306-6315.
2. “Revealing Hidden Phases and Self-Healing in Antimony Trichalcogenides and Chalcogenides.” K. B. Subila, C. P. Priyakumari, L. Houben, M. Asher, O. Yaffe, and E. Eran, *Cell Rep. Phys. Sci.* **2023**, 4, 101298.
3. “Lewis Acidity Trend of Boron Trihalides: If Not π Back-Bonding, What Else?” T. Ashith, and C. P. Priyakumari*, *ChemPhysChem* **2023**, 24, e202200761.
4. “Lewis Base/Acid Coordination Stabilizes Planar 6π Aromatic Si_6/P_6 .” C. P. Priyakumari* and Sathya S. R. R. Perumal*, *Organometallics* **2020**, **39**(16), 2951-2955.



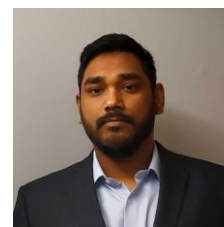
- (A) Crystal Orbital Hamilton Population diagram of Sb_2Se_3 . The plot in the inset is for longer contacts (between 3.5 Å and 4.2 Å) and indicates Sb-Sb bonding character for the bottom of the conduction band.
- (B) Raman spectra of: Sb_2Se_3 (black spectrum), after irradiation with 532 nm laser (red) and the evolution of the spectrum of the irradiated sample over time (green). The peaks that are formed at 110 and 150 cm^{-1} (red spectrum) indicate formation of elemental antimony.

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Assistant Professor

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Bioinspired Inorganic Chemistry

Profile

Ph.D – 2011-17/Indian Institute of Technology, Kanpur, India/Prof. S. P. Rath.

Postdoc – 2017-18/ICMUB, University of Burgundy, France/Prof. Claude P Gros.

Postdoc – 2019-23/University of Alabama at Birmingham, USA/Prof. Gayan B Wijeratne.

Professional Experience – 2023-Present/Assistant Professor/IISER Mohali

Research Interests

The basic theme of my research will be to comprehend the yet unclear details pertaining to several crucial biological catalytic systems by utilizing suitable model compounds, and to interrogate how such comprehension may be sensibly applied to alleviate some of the paramount challenges we face today. Numerous examples exist where model systems have pioneered fruitful biochemical research in the absence of biological insights, exhibiting the remarkable potential of bioinspired model systems. The undergraduate, masters, PhD, and postdoctoral researchers engaged in my research attempts will progress to adept in synthetic, spectroscopic, and structural approaches for tackling mechanistic ambiguities, with sound knowledge of inorganic, biological, organic, and physical chemistries, and their role in industrial/medicinal/biotechnological applications.

1. Molecular understanding of heteronuclear active sites in heme-copper oxidases:

Heme-copper oxidases (HCO) and nitric oxide reductases (NOR) catalyze the multi-electron and multi-proton reductions of O₂ and NO, respectively and each of these reactions is extremely crucial to drive cellular energy production through respiratory metabolism. However, the complexity of the structures and reactions of these native enzymes make it challenging to fully comprehend the structural features responsible for the catalytic properties of these active sites. Therefore, research idea of this work seeks to utilize synthetic mimics of HCO intermediates to gain insight into the mechanistic details and probing the reactivities of these enzymes.

2. Probing bio-inspired reactivity landscapes of heme-peroxynitrite (PN) adducts:

Heme-PN has been progressively identified as one of the strongest biological nitrating/oxidizing agents, playing roles as mediator in signal transduction pathways as well as in the disruption of cellular redox homeostasis. Hence, there is a great urgency in gaining more insight into the generation and reactivity properties of heme-PN adducts. Therefore, we intend to design the efficient modeling of the heme-PN intermediates utilizing various porphyrinic systems and explore their reactivity mechanism. Such mechanistic understanding resulting from this work will be of significance with respect to inhibitor design.

Selected Publications

(1) Pritam Mondal, Izumi Ishigami, Syun-Ru Yeh, and Gayan B. Wijeratne* The Role of Heme Peroxo Oxidants in the Rational Mechanistic Modeling of Nitric Oxide Synthase: Characterization of Key Intermediates and Elucidation of the Mechanism. *Angew. Chem. Int. Ed.* **2022**, *61*, e202211521. (Hot paper and Inside Cover)

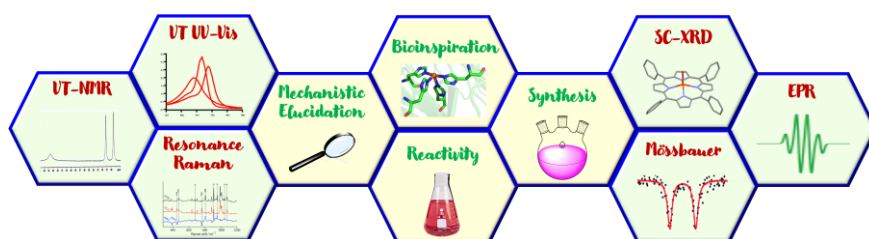
(2) Pritam Mondal, Shanuk Rajapakse and Gayan B. Wijeratne* Following Nature's Footprint: Mimicking the High-valent Heme-oxo Mediated Indole Monooxygenation Reaction Landscape of Heme Enzymes. *J. Am. Chem. Soc.* **2022**, *144*, 3843–3854. (Supplementary Cover)

(3) Pritam Mondal and Gayan B. Wijeratne* Modeling Tryptophan/Indoleamine 2,3-Dioxygenase with Heme Superoxide Mimics: Is Ferryl the Key Intermediate? *J. Am. Chem. Soc.* **2020**, *142*, 1846–1856.

(4) Pritam Mondal, Izumi Ishigami, Emilie F. Gérard, Chaeun Lim, Syun-Ru Yeh, Sam P. de Visser* and Gayan B. Wijeratne* Proton-coupled Electron Transfer Reactivities of Electronically Divergent Heme Superoxide Intermediates: A Kinetic, Thermodynamic, and Theoretical Study. *Chem. Sci.* **2021**, *12*, 8872–8883.

(5) Pritam Mondal and Sankar Prasad Rath* Cyclic Metalloporphyrin Dimers: Conformational Flexibility, Applications and Future Prospects. *Coord. Chem. Rev.* **2020**, *405*, 213117.

(6) Pritam Mondal, Sabyasachi Sarkar and Sankar Prasad Rath* Cyclic Bisporphyrin Based Flexible Molecular Containers: Controlling Guest Arrangements and Supramolecular Catalysis by Tuning Cavity Size. *Chem. Eur. J.* **2017**, *23*, 7093–7103. (Highlighted in Synfacts 2017; 13(08): 0816. DOI: 10.1055/s-0036-1590724).



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Lecturer

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Materials Chemistry

Profile:

PhD – 2015/*Indiana University, Bloomington, USA*; **Thesis:** Manipulation of the Geometric and Electronic Parameters of Metal Nanocatalysts; **Supervisor:** Professor Sara E. Skrabalak;

Professional Experience: Coordinator for Undergraduate Research and Outreach, 2015; *Indiana University, Bloomington, USA*.

Professional Experience: Assistant Professor, 2016- 2023; *GGSDS College, Chandigarh*.

Research Interests:

1. Plasmon mediated synthesis of metal nanostructures

Synthesis of designed morphologies with controlled composition is critically important in the field of nanoparticles. Their application towards catalysis, sensing and other fields can be fine-tuned with well defined morphologies. Using light sources for their synthesis can have a higher control in structure modification. The kinetics of nanoparticle synthesis can be controlled using light of various wavelength to obtain nanocrystals of defined shape.

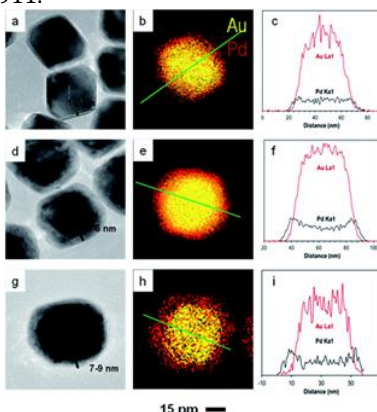
2. Nanoparticle embedded agricultural waste composite materials: a low-cost adsorbent for waste water treatment

Owing to larger surface area, nanoparticles are used as an adsorbent for the treatment of wastewater. To enhance the stability of these nanoparticles they can be supported on cheaply available agricultural waste which is also known as an adsorbent for various impurities. this nanocomposite may act as a

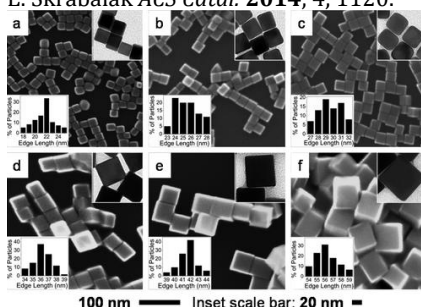
potential adsorbent for water treatment where both the support as well as the supported material play significant role towards water purification.

Publications:

(1) "A Balancing Act: Manipulating Reactivity of Shape-Controlled Metal Nanocatalysts Through Bimetallic Architecture." Moitree Laskar and Sara E. Skrabalak *J. Mater. Chem. A*, **2016**, 4, 6911.

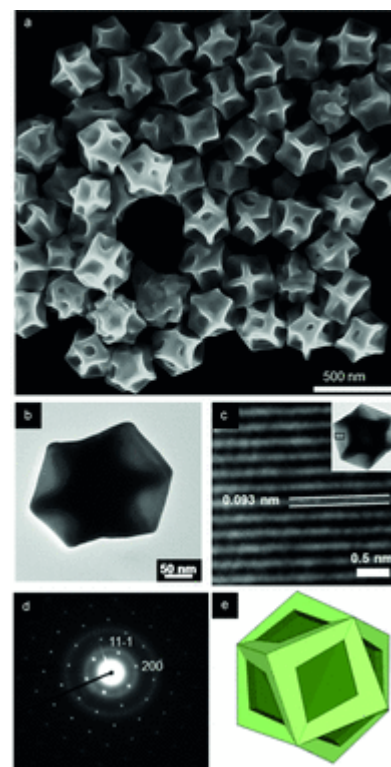


(2) "Decoupling the Geometric Parameters of Shape-Controlled Pd Nanocatalysts." Moitree Laskar and Sara E. Skrabalak *ACS Catal.* **2014**, 4, 1120.



(3) "Stereodynamics of Metal-Ligand Assembly: What Lies Beneath the 'Simple' Spectral Signatures of C2-Symmetric Chiral Chelates." Jiyoung Jung, Junyong Jo, Moitree Laskar and Dongwhan Lee *Chem. -Eur. J.* **2013**, 19, 5156.

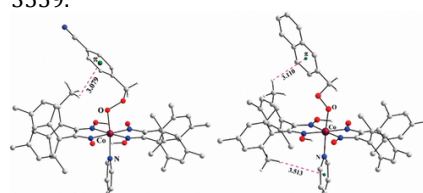
(4) "Manipulating the Kinetics of Seeded Growth for Edge-Selective Metal Deposition and the formation of Concave Au Nanocrystals." Moitree Laskar, Xiaolan Zhong, Zhi-Yuan Li and Sara E. Skrabalak *Chem Sus Chem*, **2013**, 6, 1959.



(5) "Molecular Oxygen Insertion in Benzylcobaloximes with Mixed Dioximes" Gargi Dutta, Moitree Laskar and B. D. Gupta *Organometallics* **2008**, 27, 14, 3338.

(6) "Biphenyl-Bridged Dicobaloximes: Synthesis, NMR, CV, and X-Ray Study" Mouchumi Bhuyan, Moitree Laskar and B. D. Gupta *Organometallics*, **2008**, 27, 4, 594.

(7) "Co-C Bond Reactivity and Cis Influence Relationship in Benzylcobaloximes with Glyoxime and Dimesitylglyoxime" Mouchumi Bhuyan, Moitree Laskar, Debaprasad Mandal and B. D. Gupta *Organometallics*, **2007**, 26, 14, 3559.



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Theoretical/Computational Chemistry

Profile:

Ph.D – 1972-75 Oklahoma State University, Stillwater, OK, USA.

Supervisor: Prof. Lionel M. Raff

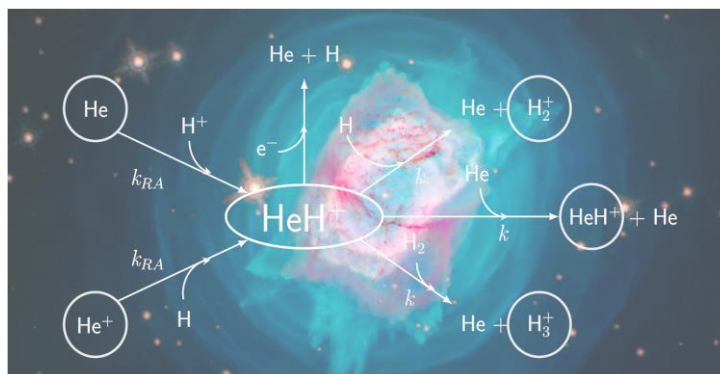
Postdoc – 1975-78/University of Toronto, Toronto, Canada

Mentor: Prof. John C. Polanyi

Professional experience – 1978-2016 IIT Kanpur;
 2007- 2017 IISER Mohali

Research Interests:

Professor Sathyamurthy's research interest has been largely focused on atoms and molecules in confined environments such as fullerenes, nanotubes, etc. In addition to determining the molecular structure of confined species, he and his associates have computed the heat capacity of such confined systems, change in the barrier for ammonia inversion, etc. He has continued interest in ion-molecule reactions that are of astrophysical interest. His recent work has focused on non-adiabatic interaction in such systems. He and his collaborators have been exploring the utility of artificial neural works in fitting ab initio potential energy surfaces in multiple dimensions and following these studies, investigating energy transfer between molecular species in interstellar media. Along with the undergraduate students at IISER Mohali, he has discovered synchronous pulsed flowering in Passionflower and examined the underlying nonlinear dynamics. In addition, they have also examined the possible mechanism for pattern formation in the same flower.



Selected Publications:

(1) Heat capacity of endohedral fullerenes, $Rg@C_{60}$ ($Rg = \text{He, Ne, Ar and Kr}$), A. Koner, C. Kumar and N. Sathyamurthy, Mol. Phys. (M. Baer Festschrift), 116, 2728-2735 (2018).

(2) Synchronous pulsed flowering in *Passiflora incarnata*, S. Goyal, R. Reji, S. S. Tripathi and N. Sathyamurthy, Current Science, 117, 1211-1216 (2019).

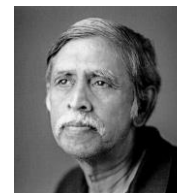
(3) Non-adiabatic coupling and conical intersection(s) between potential energy surfaces for HeH_2^+ , A. K. Gupta, V. Dhindhwal, M. Baer, N. Sathyamurthy, Satyam Ravi, S. Mukherjee and B. Mukherjee, S. Adhikari, Mol. Phys. 2020, 118:e1683243

(4) Effect of confinement on ammonia inversion, S. Mallick, P. Kumar, B. K. Mishra and N. Sathyamurthy, Eur. Phys. J. D (2021) 75:113.

(5) HeH^+ Collisions with H_2 : Rotationally Inelastic Cross Sections and Rate Coefficients from Quantum Dynamics at Interstellar Temperatures, K. Giri, L. González-Sánchez, R. Biswas, E. Yurtsever, F. A. Gianturco, N. Sathyamurthy, U. Lourderaj, and R. Wester, J. Phys. Chem. A 126, 2244–2261 (2022).

(6) Rotational state-changes in C_5N^- by collisions with He and H_2 , R. Biswas, K. Giri, L. González-Sánchez, F. A. Gianturco, N. Sathyamurthy, U. Lourderaj, E. Yurtsever, and R. Wester, MNRAS, 522, 5775-5787 (2023).

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Matrix Isolation Infrared Spectroscopy

Profile:

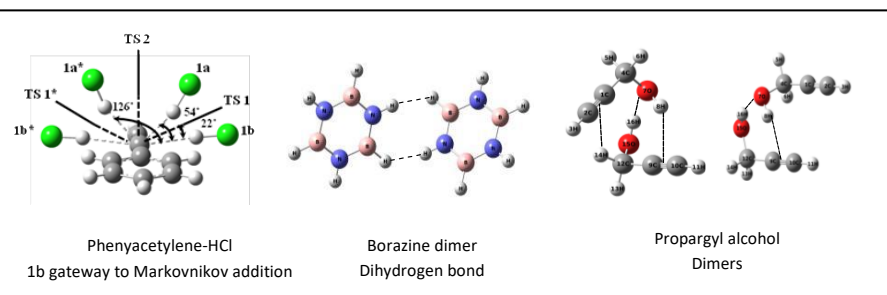
Ph.D – 1983/Vanderbilt University, USA
 Supervisor: Prof. Joel Tellinghuisen
Postdoc–1983-85/Indiana Univ. USA
 With Prof. James P Reilly
Professional experience (1986-2011)
 IGCAR, DAE, Kalpakkam, India

Matrix Isolation Spectroscopy

A cold isolated molecule technique where molecules under study are trapped in a cryogenic matrix of an inert gas, such as Ar or N₂, for eventual study by infrared spectroscopy. Using this technique, non-covalent interactions and molecular conformations are studied.

Past group members: Dr. Bishnu P Kar, Dr. Anamika (Postdocs), Dr. Ginny, Dr. Kanupriya, Dr. Jyoti, Dr. Pankaj (PhD researchers), Mr. Mrinal, Mr. Gaurav, Dr. Kapil, Mr. Deepak, Ms. Mariyam, Mr. Piyush, Dr. Akshay, Ms. Gargi, Mr. Srijit, Ms. Shruti, Mr. Ravi, Mr. Sumit, Ms. Priyanka, Ms. Divita, Ms. Amala, Ms. Shivangi, Ms. Dipali, Ms. Himanshi, Mr. Jai Khatri (Masters researchers).

Non-Covalent Interactions: The study of hydrogen-bonded interactions is an important area of research. We study the competition between the different isomers of hydrogen-bonded complexes, involving precursors that can potentially serve as both hydrogen bond acceptors and donors. One such competition involves that between n-σ* and H-π contacts. In many of the systems, our matrix isolation experiments identified both global and local minima. One of the highlights of our work is discerning the role played by weak C-H...O interactions in stabilizing hydrogen bonded complexes in phenylacetylene-water system. In the phenylacetylene-HCl complex, we identified the role of an H-π complex as the gateway for Markovnikov addition. We have also studied a number of hydrogen bonded complexes involving π systems, of phenylacetylene, acetylene,



borazine, and benzene and have identified both global and local minima in these systems. In one of these studies, we experimentally observed a dihydrogen bonded complex, for the first time in a non-metal hydride system.

Study of propargyl alcohol and propargyl amine highlighted the *interplay of interactions* in complexes with *multiple* contacts. Propargyl alcohol dimers were also studied, that has relevance in astrochemistry.

Conformations: We also study the conformations of amino acids. In addition to experimentally observing various conformers, we also try to understand the basic backbone structures adopted by the amino acids and the reasons for conformational preferences in amino acids.

We are also interested in halogen bonding interactions.

Selected Publications

- (1) "Do Amino Acids Prefer Only Certain Backbone Structures? Steering through the Conformational Maze of L-Threonine" Pankaj Dubey, M. Anamika Mukhopadhyay, K. S. Viswanathan, *J. Mol. Struct.* **2019**, 1175,117
- (2) "From Propargyl Alcohol-Water to the Propargyl Alcohol Dimer: Where does the Propargyl Alcohol-Methanol fit in?" Jyoti Saini, K. S. Viswanathan, *New J. Chem*, **2019**, 43, 3969
- (3) "Multiple Hydrogen Bond Tethers for the Grazing Formic Acid in its Complexes with Phenylacetylene", Ginny Karir, Gaurav Kumar, Bishnu Prasad Kar, K. S. Viswanathan, *J. Phys. Chem. A*, **2018**, 122, 2046

- (4) "A Tale of Two Structures: Stacks and Ts of Borazine and Benzene Hetero and Homo Dimers", Kanupriya Verma, K. S. Viswanathan, *Chemistry Select*, **2018**, 3, 864

- (5) "How different is the borazine-C₂H₂ dimer from the C₆H₆-C₂H₂ dimer?" A matrix isolation infrared and ab initio study" Kanupriya Verma, K.S. Viswanathan, Moumita Majumder, N. Sathyamurthy *Mol. Phys.* **2017**, 115, 2637.

- (6) "The Borazine Dimer: The Case of Dihydrogen Bond Competing with Classical Hydrogen Bond", Kanupriya Verma, K. S. Viswanathan, *Phys. Chem. Chem. Phys.* **2017**, 19, 19067

- (7) "H-π Landscape of Phenylacetylene-HCl System: Does this Provide the Gateway to the Markovnikov Addition" complex" Ginny Karir, K. S. Viswanathan, *J. Phys. Chem. A*, **2017**, 121, 5797

- (8) "The elusive n-σ* complex in the hydrogen bonded systems of phenylacetylene" Ginny Karir, Mariyam Fatima, K. S. Viswanathan, *J. Chem. Sci.* **2016**, 128, 1557

- (9) "Does a Hydrogen-Bonded Complex with Dual Contacts Show Synergism" Jyoti Saini, K.S. Viswanathan, *J. Mol. Struct.*, **2016**, 1118, 147

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Inorganic and Coordination Chemistry

Profile:

PhD – 1968/McMaster University, Canada; **Supervisor:** Professor R. J. Gillespie, FRS.

Research Associate: - 1980-81 & 1986-87; McMaster University/Professor R. J. Gillespie, FRS

Visits: Indo-Canadian exchange Program – 1990/University of New Brunswick, Fredericton.

2000/University of Bremen/DFG

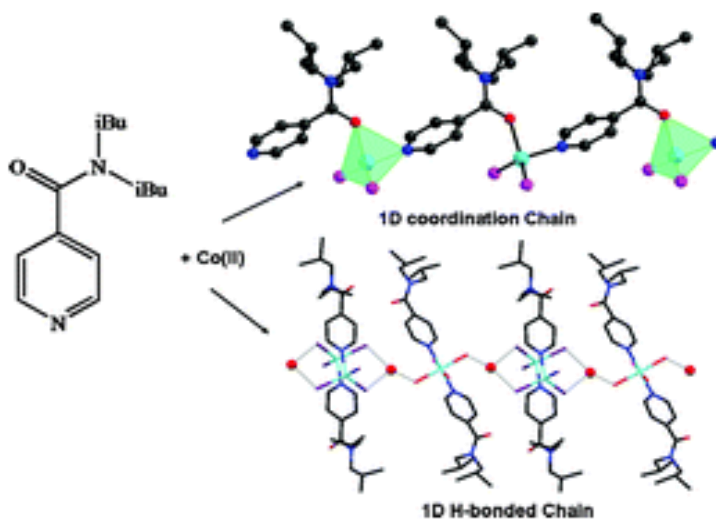
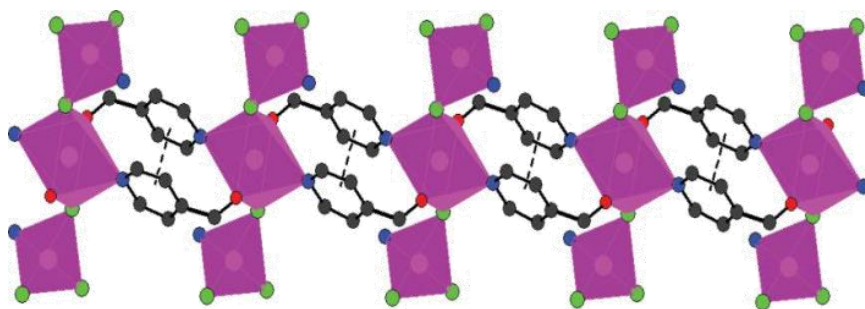
Professional Experience: 1970 – 2005 / Professor/Panjab University.

2007 – 2016: Professor/IISER Mohali.

Research Interests:

Coordination driven and/or H-bonded 1D, 2D and 3D frameworks of metal complexes of pyridyl- and pyrazinyl-N,N-disubstituted carboxamides

A class of transition metal complexes which are exclusively investigated for their crystal structure because they self assemble in their crystal lattice to form interesting 1D/2D and 3D coordination frameworks. We have been interested in developing acyclic ligands containing pyridyl and pyrazinyl carboxamides and thiocarboxamides functionalities. The presence of transition metal ions has added a new dimension to the creation of functional materials. The varied coordination geometries adopted by the metal centres guide the direction of propagation of the network resulting in frameworks with exciting topology. These ligands contain efficient metal coordination sites with H-bonding functionalities and are an ideal choice since they have the structural



adaptability for both hydrogen bonding as well as coordination polymerization.

Selected Publications:

(1) P. Kapoor, A. P. S. Pannu, G. Hundal, R. Kapoor, M. Corbella and N. Aliaga-Alcalde, M. S. Hundal. *Dalton Trans.* **2010**, 39 7951-7959.

(2) P. Kapoor, A. P. S. Pannu, M. Sharma, G. Hundal, R. Kapoor and M. S. Hundal. *J. Coord. Chem.* **2011**, 64, 56-271.

(3) A. P. S. Pannu, P. Kapoor, G. Hundal, R. Kapoor, M. Martinez-Ripoll,

M. S. Hundal, *J. Coord. Chem.* **2011**, 64, 1566-1577.

(4) A. P. S. Pannu, M. Martinez-Ripoll, R. J. Butcher and M. S. Hundal, *Polyhedron*, **2011**, 30, 1691- 1702.

(5) A. P. S. Pannu, P. Kapoor, G. Hundal, R. Kapoor, M. Corbella, N. Aliaga- Alcalde and M. S. Hundal *Dalton Trans.* **2011**, 40, 12560-12569.

Honorary / Visiting / Adjunct Faculty



Dr. N. Sathyamurthy

Honorary Professor & Founder Director,
IISER Mohali, SAS Nagar -140306.
E- mail: nsath@iisermohali.ac.in
Period: July 2020 – Present



Dr. Gautam R. Desiraju

Professor Emeritus
Solid State and Structural Chemistry Unit
Indian Institute of Science, Bangalore - 560012
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Telephone: +91 44 2257 4220
Period: October 2020 – Present



Dr. Ramasamy Murugavel

Professor
Department of Chemistry
IIT Bombay, Mumbai – 400076
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Telephone: +91 22 2576 7151
Period: October 2020 – Present



Dr. Souvik Maiti

Director & Chief Scientist
CSIR-IGIB,
Sukhdev Vihar, Mathura Road, New Delhi - 110 025
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Telephone: 91-11-29879108
Period: October 2020 – Present



Dr. S. Keshavamurthy

Professor
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Telephone: +91-512-2597043
Period: August 2020 – July 2021

Honorary / Visiting / Adjunct Faculty



Dr. J. Narasimha Moorthi

Professor
Department of Chemistry
IIT Kanpur, Kanpur – 208 016
E- mail: moorthi@iitk.ac.in
Telephone: +91 512-2597438
Period: October – December 2007
Course taught: Chemistry of Elements & Chemical Transformations



Dr. Ram Mohan

Wendell and Loretta Hess Professor of Chemistry
Department of Chemistry,
Illinois Wesleyan University, Bloomington, IL 61701 USA
E- mail: rmohan@iwu.edu
Telephone: +1 309-556 3829
Period: October – December 2012, October 2015, August 2016 & August 2017
Course taught: Green Chemistry



Dr. Michael Baer

Professor
The Fritz Haber Center for Molecular Dynamics
18 B Nahalat Yitzhak Street, Apt 15167448, Tel Aviv, Israel.
E-mail: michaelb@fh.huji.ac.il
Telephone: +972-3-6955678
Period: August 2013 – December 2013
Course taught: Non-adiabatic Transitions



Dr. Mangala Sunder Krishnan

Professor
Department of Chemistry
IIT Madras, Chennai – 600 036
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Telephone: +91 44 2257 4220
Period: January – April 2014
Course taught: Energetics and dynamics of chemical reactions



Dr. Sumit Bhaduri

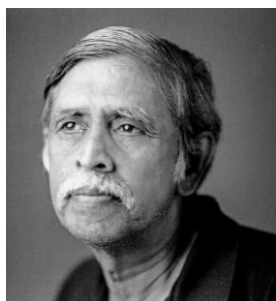
Formerly Senior Scientific Advisor (Reliance Industries Limited)
Retired Visiting Professor (North Western University, USA)
Retired Adjunct Professor (IIT Bombay).
E- mail: bhaduri.sumit@gmail.com
Period: August – December 2016
Course taught: Materials chemistry

Former Faculty



Prof. Ramesh Kapoor

Professor (Retired)
E-mail: rkapoor@iisermohali.ac.in
Telephone: +91 9815247070
Period: 2007 – 2016
Research Area: Inorganic and Coordination Chemistry



Prof. K. S. Viswanathan

Professor (Retired)
E-mail: ksvish53@gmail.com
Telephone: +91 9530802088
Period: 2011 – 2019
Research Area: Matrix Isolation Infrared Spectroscopy
Current Position: Visiting Professor at Krea University



Dr. Monika Sharma

INSPIRE Faculty
E-mail: monika.sharma@plaksha.edu.in
Telephone: +91 7087543458
Period: 2015 – 2020
Research Area: Computational Biophysical Chemistry
Current Position: Associate Professor at Plaksha University, Punjab



Dr. Debrina Jana

INSPIRE Faculty
E-mail: deprina.chem@gmail.com
Telephone: +91 7744029918
Period: 2016 – 2020
Research Area: Computational Biophysical Chemistry
Current Position: Assistant Professor at Gour Mohan Sachin Mandal Mahavidyalaya, West Bengal.



Dr. Bimalendu Adhikari

INSPIRE Faculty
E-mail: adhikarib@nitrkl.ac.in
Period: 2016 – 2018
Research Area: Molecules to Materials
Course taught: Materials chemistry, Bio-Organic Chemistry
Current Position: Assistant Professor at NIT Rourkela, Odisha.

Conferences/Meetings organized

Junior National Organic Symposium Trust (J-NOST) Conference:

The 7th Junior National Organic Symposium Trust (J-NOST) Conference organized by IISER Mohali and NOST was held at IISER Mohali during 15-18th Dec 2011. Many research scholars from India and the United Kingdom participated in the conference. The conference was inaugurated by Prof. N. Sathyamurthy (Director, IISER Mohali), Prof. Vinod K. Singh (Chairman, NOST and Director, IISER, Bhopal) and Prof. G.S.R. Subba Rao (Chairman, NOST Board of Trustees). There were 60 oral presentations and 34 poster presentations. In addition, there were three plenary lectures by Prof. T. K. Chakraborty (Director, CDRI Lucknow), Prof. Sandeep Verma (IIT Kanpur) and Prof. Javed Iqbal (Director, ILS Hyderabad).

Co-Conveners: Dr R. Vijaya Anand and Dr S. Arulananda Babu

3rd Inter IISER Chemistry Meet

Since 2008 an Inter IISER Chemistry Meet is organized each year to bring all people in Chemistry together to share research activities of various groups through oral and poster presentations. First and second such meet was organized by IISER Pune and IISER Kolkata, respectively. In 2011, IISER Mohali hosted the 3rd Inter IISER Chemistry Meet during February 20-21, at its new campus. This meet focused on the current status and future projections of research in various fields of Chemistry and related areas. In this meet oral (26) and poster (9) presentations by various faculties and students showcased the interdisciplinary research activities in the five premier institutes of India. Through these presentations it was expected to have exchange of ideas for generating scope for collaborations as well as to give an opportunity to young minds to interact with others. 2011 is the International Year of Chemistry and thus it was a great opportunity to celebrate it together.

Convener: Dr. Sanjay Mandal

Indo-German Conference on Modelling Chemical and Biological (Re)Activity (MCBR3)

The third Indo-German conference on modelling chemical and biological (re)activity (MCBR3) was jointly organized by IISER and NIPER during 26 Feb to 1 Mar, 2013. The conference brought together several research scholars from India and Germany working on computational modelling of chemical reactivity and biological activity. The conference included several oral presentation and plenary lectures by Prof. E. D. Jemmis (IISER Trivendram), Prof. Walter Thiel (MPI Mulheim), Prof. Peter Comba (Univ Heidelberg) and Prof. G. N. Sastry (IICT Hyderabad). A large number of student researchers across the country attended and presented their works at three poster sessions. They were also benefited from training session lectures by experts on chosen advanced topics. A special Science Day lecture was given by Prof. Gernot Frenkling (Univ Marburg). The concluding day the conference was held at IISER Mohali campus. The conference also featured a cultural event jointly put together by the students of NIPER and IISER.

Conveners: Dr. P. V. Bharatam (NIPER) and Dr. K. R. Shamasundar (IISER, Mohali)

History of Chemistry in India

A seminar on "History of Chemistry in India" was held at IISER Mohali on 15, November, 2013. Welcome address was delivered by Prof. R Gadagkar, FNA, Chairman, Research Council for History of Science, INSA, followed by remarks by Prof. N Sathyamurthy, FNA, Director, IISER, Mohali and Prof. Krishan Lal, FNA, President, INSA, IISER Mohali. The talks traced the development of chemistry in the country over many decades.

National Seminar on Crystallography (NSC43A)

The National Seminar on Crystallography (43A) (an early event of Indian Crystallographic Association) was held in Indian Institute of Science Education and Research Mohali during 28 - 30 March, 2014. The year 2014 has been celebrated as the International Year of Crystallography (IYCr2014) to mark 100 years since the award of Nobel Prize to Max von Laue for the discovery of X-ray diffraction by crystals. This national seminar at IISER Mohali was the first of the three national seminars held in India in 2014 to mark IYCr2014. The seminar was attended by about 100 participants (professors, post-doctoral fellows, PhD students and MS students) from various parts of the country. The scientists, post-docs and the students working in the different areas of crystallography in the country presented their exciting results through plenary lectures, other oral presentations and poster sessions and exchanged their idea to enrich their view and knowledge. The conference had equal balance on oral and poster presentations in the areas of macromolecule and small molecule crystallography and the application of crystallography in materials science. The conference was organized with the generous funding from IISER Mohali, industrial sponsor and through the registration fee from the participants.

Organizers: Dr. Angshuman Roy Choudhury (Chairman) and Dr. Sanjay Singh (Convener) and all other DCS members in various capacities.

Conferences/Meetings organized

Advances in Applications of Transmission Electron Microscope

A workshop dedicated to latest developments on applications of transmission electron microscope was organized on 24th July, 2015. Prof. N. Sathyamurthy, FNA, Director, IISER-Mohali inaugurated the workshop with his opening remarks. Keynote lectures were delivered by Prof. Ashok Ganguli, (Director, INST, Mohali), Prof. N. Ravishankar (MRC, IISc, Bangalore) and Prof. Ranjan Datta (JNCASR, Bangalore). The talks emphasized the nature and the usefulness of data acquired with TEM accessories for various research purposes.

Organizer: Dr. Ujjal K. Gautam

24th National Conference on Liquid Crystals

The 24th NCLC was organised by the Indian Institute of Science Education and Research (IISER) Mohali, Punjab in association with the Indian Liquid Crystal Society (ILCS) during 11–13 October 2017. Dr. Santanu Kumar Pal, Department of Chemical Sciences conducted the 3-day conference guided by the National Advisory Board and supported by an Organising Committee. The conference was attended by about 200 participants consisting of senior researchers and young Ph.D. students from various institutes and universities across India as well as some from abroad. The conference was aimed at serving as a platform for stimulating and collaborative discussions among the young and senior researchers working in this interdisciplinary field of liquid crystals (LC) in a less formal environment. The scientific programme was designed in order to cover a variety of fundamental and applied topics in LCs and related soft matter. Nine technical sessions were conducted including a Keynote Address, 23 Invited Lectures (IL), 25 Oral Presentations (OP) and 85 Poster Presentations (PP). Scientists from India, UK, Ireland and so on delivered Invited talks covering topics such as the structural parameters of two nematic phases, twist-bend nematic phase, discovery of triphenoxazoles, ferroelectric LCs to mention a few. The poster presentations were conducted on the first day itself. The participants in the poster session included undergraduates, graduate students, research scholars and post-doctoral fellows. The private sponsors like Anton Paar, Edwards, IKA, Borosil, Sinsil International, Xenocs and TCI chemicals put up exhibition stalls for 3 days with an interactive approach with the delegates.

Organizers: Dr. Santanu Kumar Pal (Convener) and Dr. Arijit Kumar De and Dr. Ujjal K. Gautam (Co-Conveners) and all other DCS members in various capacities.

16th Discussion meeting on Spectroscopy and Dynamics of Molecules and Clusters (SDMC2019)

SDMC2019 meeting was held in Koti resorts Shimla, India during 21-24 February, 2019. An annual discussion meeting and conference that brings together experimental, theoretical spectroscopists and dynamicists from India and abroad. The focus is on extended talks followed by invigorating discussions during poster sessions. The meeting is usually held in a resort, a place that is slightly off the road from the usual crowd. This time the annual meeting in February 2019 was jointly organized by a Indian Institute of Science Education and Research (IISER) Mohali and Indian Institute of Technology (IIT) Kanpur at the Koti Resort, Shimla.

Organiser(s): Dr Balanarayan P, Dr Arijit K De, Dr Sugumar V, Prof K S Viswanathan, Prof K Srihari (IIT Kanpur)

Recent Advances in Organic and Bioorganic Chemistry (RAOBC) symposium

This symposium provided an excellent platform to dynamic researchers in organic, bioorganic and medicinal chemistry to share their innovations. This was a proud occasion for the department and the institute to host some of the most well-known and influential voices in synthetic organic chemistry. This was held during 22-24, March 2019.

Organiser(s): Chairman: Dr. S. Arulanda Babu; Convener: Dr. S. S. V. Ramasastry; Co-conveners: Dr. R. Vijaya Anand & Dr. Sugumar Venkataramani

First edition of the CRIKC Chemistry Symposium (CCS-2019)

A milestone event of the first edition of the CRIKC Chemistry Symposium (CCS-2019) was held at IISER Mohali during 2,3 Nov 2019 and it was organized by the department of chemical sciences, IISER Mohali along with IIT Ropar, Panjab University, INST Mohali and NIPER Mohali.

Conveners: Prof. K. N. Singh, Panjab University, Chandigarh, Dr. T. J. Dhilip Kumar, IIT Ropar, Dr. Kamalakannan Kailasam, INST Mohali, Dr. Sankar K. Guchhait, NIPER Mohali, Dr. Rohit Kumar Sharma, Panjab University, Chandigarh.

Treasurers: Dr. Sabyasachi Rakshit, IISER Mohali Dr. Kamalakannan Kailasam, INST Mohali.

Conferences/Meetings organized

Chemistry at the Interface of Light, Matter, and Life

One-day virtual meeting on the theme “Chemistry at the Interface of Light, Matter and Life” on the event of Chem Day 2020, IISER Mohali, 17th October 2020. The purpose of this event was to bring together an active group of scientists to share their insights in the rapidly growing diversities in Chemistry

Organizer: Dr. Sabyasachi Rakshit, Dr. Ujjal K. Gautam and Dr. Arijit K De.

29th CRSI-NSC & CRSI-ACS symposium series

The 29th CRSI National Symposium in Chemistry (CRSI-NSC) and CRSI-ACS Symposium series was organized by the Department of Chemical Sciences between July 07-09, 2022. The symposium had several CRSI medal lectures, CRSI Award, and CRSI-ACS lectures, including special lectures on Women in Chemical Sciences. Around 550 participants including eminent scientists, young scientists, and researchers attended it. Nearly 320 posters were presented by student participants and 30 poster awards were given. Organizers: Dr. Sanjay Singh; Co-convener: Dr. R. Vijaya Anand.

Courses offered by the Department

Core year courses for BS-MS Programme

Course Number	Title	Credits
CHM101	Basic inorganic chemistry	3
CHM111	Chemistry lab I	1
CHM102	Basic organic chemistry	3
CHM112	Chemistry lab II	1

Pre-major year Courses for BS-MS Programme

CHM201	Introduction to spectroscopic methods	3
CHM202	Chemical thermodynamics	2
CHM211	Chemistry lab III	2
CHM203	Chemical kinetics	3
CHM204	Electrochemistry, colloids and interfaces	3
CHM212	Chemistry lab IV	2

3rd year mandatory courses for BS-MS Programme

CHM301	Quantum chemistry I	4
CHM302	Organic chemistry – reactions and mechanism	4
CHM303	Main group chemistry	4
CHM311	Organic chemistry lab	4
CHM304	Quantum chemistry II	4
CHM305	Physical organic chemistry	4
CHM306	Transition metal chemistry	4
CHM312	Inorganic chemistry lab	4

4th year mandatory courses for BS-MS Programme

CHM401	Molecular spectroscopy	4
CHM402	Chemistry of materials	4
CHM411	Physical chemistry lab	4
CHM403	Analytical chemistry	4
CHM404	Statistical thermodynamics	4
CHM412	Analytical chemistry lab	4

IDC courses

IDC30X/CHM30X**	Symmetry in chemistry	4
IDC4XX/CHM6XX**	Selected Analytical Techniques in organic chemistry	4
	Seminar (attending)	1
	Seminar (Delivering)	1
	Seminar (Delivering)	2

Courses offered by the Department

Elective and PhD Courses

Course Number	Title	Credits
CHM601	Advanced inorganic chemistry	4
CHM602	Magnetic resonance	4
CHM604	Advanced organic chemistry	4
CHM606	Bio-organic and medicinal chemistry	4
CHM607	Chemical crystallography	4
CHM608	Advanced industrial chemistry	4
CHM609	Polymer chemistry	4
CHM610	Chemistry of natural products	4
CHM611	Frontiers of organometallic chemistry	4
CHM612	Asymmetric synthesis and catalysis	4
CHM613	Supramolecular chemistry	4
CHM615	Kinetics and dynamics of chemical reactions	4
CHM616	Theoretical and computational chemistry	4
CHM617	Chemical dynamics and non-adiabatic interactions	4
CHM618	Bioinorganic chemistry	4
CHM619	Numerical methods in chemistry	4
CHM621	Advances in X-ray crystallography and its applications	4
CHM622	Chemistry, Energy and Environment	4
CHM623	Concepts in nanomaterials and chemical applications	4
CHM624	Soft matter, colloids and interfacial phenomena	4
CHM626	Photochemistry – concepts, techniques and applications	4
CHM627	Molecular Spectroscopy	4
CHM628	Statistical thermodynamics	4
CHM629	Magnetochemistry	4
CHM6XX**	Inorganic polymers, rings, macrocycles and cages	4
CHM6XX**	Contemporary main group chemistry	4
CHM6XX**	Spectroscopic methods for inorganic chemistry	4

**Course numbers yet to be assigned

Research and Teaching Facilities

Central Facilities

- ❖ Bruker Avance III 600 MHz NMR
- ❖ Bruker Avance III 400 MHz NMR
- ❖ Waters SYNAPT G2S High-Definition Mass Spectrometer – with ESI, APCI, ESCI, ASAP and MALDI Ion sources and TOF detector Coupled with UPLC/nano-UPLC and AP-GC
- ❖ Rigaku Ultima IV powder X-ray diffractometer
- ❖ Bruker AXS KAPPA APEX II Single Crystal X-ray Diffractometer with variable temperature Oxford Cryosystem 700 Series
- ❖ Renishaw laser Raman spectrometer
- ❖ Fully automated Xeuss SAXS/WAXS System (Model C HP100 fm)
- ❖ Jeol Field emission scanning electron microscope with EDS facilities

Departmental Research Lab Facilities

- ❖ Bruker 400 MHz NMR (DST-FIST Facility)
- ❖ Agilent Cary 5000 UV-Vis-NIR Spectrophotometer
- ❖ SHIMADZU GC-2010 Plus Gas Chromatograph with AOC-20i Autoinjector and AOC-20s Auto sampler
- ❖ PerkinElmer DSC8000 Differential Scanning Calorimeter with Controlled Liquid Nitrogen (CLN2) accessory
- ❖ PerkinElmer Spectrum RX1 FT-IR Spectrometer
- ❖ SHIMADZU DTG-60H Simultaneous DTA-TGA Apparatus
- ❖ Anton Paar Monowave 300 Microwave Synthesis Reactor
- ❖ Mbraun MB-SPS Solvent drying unit
- ❖ Waters 515 Semi-Preparative High-Performance Liquid Chromatography with 2707 Autosampler and 2998 Photo Diode Array detector
- ❖ Anton Paar MCP 300 Polarimeter
- ❖ Leco TruSPEC CHNS analyzer
- ❖ Scanvac Lyophilizer

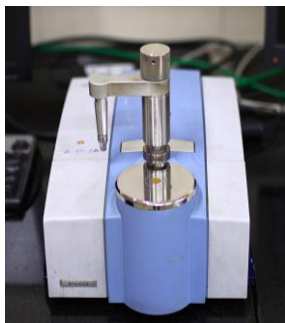
Departmental Teaching Lab Facilities

- ❖ ANTON PAAR Raman Spectrometer Model-CORA2700 (1 No)
- ❖ LABINDIA AA7000 Atomic Absorption Spectrophotometer (1 No)
- ❖ LABINDIA UV-Vis Spectrophotometer (8 Nos)
- ❖ Perkin Elmer Spectrum Two FT-IR spectrometer (3 Nos)
- ❖ Magritek Spinsolve benchtop NMR spectrometer (1 No)
- ❖ Bruker Alpha FT-IR spectrometer (2 Nos)
- ❖ SHIMADZU Model RF-5301 PC Spectrofluorophotometer (1 No)
- ❖ SHIMADZU Model RF-6000 Spectrofluorophotometer (1 No)
- ❖ Rigaku XtaLAB mini-Desktop X-ray diffractometer with Oxford cryosystem (1 No)
- ❖ Oz-Air Ozonolysis apparatus

Computational and Theoretical Chemistry Facilities (Central facilities)

- ❖ High-performance computing cluster: 2 x Intel(R) Xeon(R) Gold 6230R CPU @ 2.10GHz with a total of over 1872 processor cores, 49 Nodes (2 Master Nodes + 39 Compute Nodes + 2 login Nodes + 2 Database Nodes + 3 Storage Nodes) with global storage of 2 x 102 TB and a system memory of 384GB (CPU) & 768GB (GPU)

Research and Teaching Facilities



The new miniaturized Bruker Alpha FT-IR spectrometer



Leco TruSPEC CHNS analyzer



Magritek Spinsolve benchtop NMR spectrometer



Anton Paar MCP 300 Polarimeter

Research and Teaching Facilities



PerkinElmer DSC8000 Differential Scanning Calorimeter with Controlled Liquid Nitrogen



SHIMADZU RF-6000 Spectrofluorophotometer



High-Performance Liquid Chromatography with 2707 Autosampler and 2998 Photo Diode Array detector

Perkin Elmer Spectrum2 FT-IR spectrometer



Research and Teaching Facilities



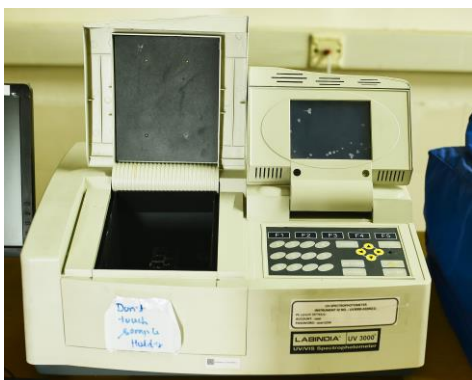
Anton Paar Monowave 300 Microwave Synthesis Reactor



ANTON PAAR Raman Spectrometer CORA2700



Agilent Cary 5000 UV-Vis-NIR Spectrophotometer



LABINDIA UV-Vis Spectrophotometer



SHIMADZU Simultaneous
DTA-TGA Apparatus

Research and Teaching Facilities



Rigaku XtaLAB mini-Desktop
X-ray diffractometer with
Oxford cryosystem



Bruker 400 MHz NMR (DST-FIST Facility)

Alumni Placements

Chemistry major (MS) students

Name	Batch	Current Position
Amita Agarwal	MS07	Process Researcher at Shell India
Mrinal Shekhar	MS07	PhD at University of Illinois at Urbana-Champaign
Shalender Jain	MS07	Lecturer at Govt. College Haryana
Gaurav Kumar	MS08	PhD at University of Southern California, USA
Kapil Dave	MS08	PhD at University of Illinois, Urbana-Champaign, USA
Asif Iqbal	MS08	PhD at Aarhus university, Denmark and TIFR Mumbai
Vinod Kumar	MS08	PhD at IISER Mohali
Sumit Mittal	MS08	PhD at Max Planck Institute for Coal Research, Germany
Deepansh Shrivastava	MS08	PhD at Ohio State university, USA
Manish Pareek	MS08	PhD at TU Berlin, Germany
Mariyam Fatima	MS09	PhD at Max Planck Institute of Structure and Dynamics of Materials, Germany
Nishtha Agarwal	MS09	PhD at Cardiff Catalysis Institute, UK
Deepak Verma	MS09	PhD at University of Southern California, USA
Karan Pratap Singh Yadav	MS09	MBA from IIM Calcutta, India
Jyoti Saini	MS09	PhD at IISER Mohali, India
Indu Verma	MS09	PhD at IISER Mohali, India
Priyanka Dogra	MS09	PhD at IISER Mohali, India
Agastya P. Bhati	MS09	PhD at University College London, UK
Aditya Jhaharia	MS09	PhD at École Normale Supérieure, Paris
Gaurav Verma	MS09	PhD at University of South Florida, USA
Yash Maurya	MS09	MBA from School of Petroleum Management, Gandhinagar
Sudeep Maheshwari	MS09	ABN Bank, Netherlands
Shiv Charan Dudi	MS09	Lecturer at Allen Career Institute, Kota, India
D. Jeiyendra Pradeep	MS10	PhD at TIFR, Mumbai/University of Lille 1, France
Vipin T.Raj	MS10	PhD at National Centre for Earth Science Studies
Anubhuti Singh	MS10	PhD at Technische Universität München, Germany
Ravi Ranjan	MS10	PhD at NCL Pune
Bharti Kumari	MS10	PhD at Technische Universität Darmstadt, Germany
Piyush Mishra	MS10	PhD at Purdue University, USA
Pratip Chakraborty	MS10	PhD at Temple University, USA
Jagadish Prasad Hazra	MS10	PhD at IISER Mohali, India
Ashish Kumar	MS10	PhD at IISER Mohali, India
Ankur Kumar Gupta	MS10	PhD at Indiana University, USA
Jagdale Gargi Satishraj	MS10	PhD at Indiana University, USA
Lilit Jacob	MS10	PhD at University of New South Wales, Canberra, Australia
Harshita Pawar	MS10	Development Editor at ACS, New Delhi, India
Haseeb Hakkim	MS10	PhD at IISER Mohali, India
Arya J. S	MS10	PhD at CSIR-NIIST, Kerala
Raut Akshay Hemant	MS10	PhD at Ruhr University of Bochum, Germany
Rupali Chawla	MS10	PhD at Rutgers University, USA
Prerna Paliwal	MS10	PhD at Weizmann Institute of Science, Israel
Prashant Singh	MS10	PhD at IISER Mohali, India
Rajat Garg	MS10	PhD at IISER Mohali, India
Upakul Sarma	MS10	Junior Administrative Assistant at Assam Secretariat
Aneeshma Peter	MS10	PhD at University of Quebec at Trois-Rivieres, Canada
Akhil V Gopal	MS10	PhD at IISER Kolkata
Ankit Kumar Agrawal	MS10	PhD at CSIR-IIP, Dehradun
Soniya Rani	MS10	PhD at NCL Pune
Nitish Kumar	MS10	Preparing for IAS and Bank exams
Nitin Kumar Singh	MS10	PhD at IISER Mohali, India

Alumni Placements

Chemistry major (MS) students

Name	Batch	Current Position
Shweta Sreenivasan	MS11	PhD at Massachusetts Institute of Technology, USA
Nakul Thete	MS11	PhD at Virginia Tech University, Virginia, USA
Srijit Mukherjee	MS11	PhD at University of Colorado, Boulder, USA
Justin K. Thomas	MS11	PhD at Ohio state University, Columbus
Lakshmi Bhai N. V.	MS11	PhD at Ohio State University, USA
Manisha	MS11	PhD at University of Massachusetts, Amherst, USA
Jopaul Mathew	MS11	Virginia Tech University, USA
Abhinay Vardhan	MS11	PhD at IISER Mohali
Sandhya Singh	MS11	PhD at University of Otago, New Zealand
Anjali Mahadevan	MS11	PhD at IISER Mohali
Athira T. John	MS11	Ph. D. at IISER Trivandrum
Sruthi Mohan	MS11	Ph. D. at University of Illinois, Chicago, USA
Akshey Sandhu	MS11	Probationary officer, SBI
Manmohan	MS11	Geeta Tutorials Career Academy
Yengkhom Sunanda	MS11	Preparing for Civil Services in Delhi
Rohit Kumar Patidar	MS11	Allen Career Institute, Kota/Indore
Vaishali	MS11	PhD at Institute of Energy and Climate Research, Julich, Germany
Aman Kumar Bhonsle	MS11	PhD at Indian Institute of Petroleum, Dehradun
Neeru Mittal	MS12	Ph. D. at ETH Zurich, Switzerland
Aayush	MS12	PhD at Purdue University, USA
Satavisa Jana	MS12	PhD at UCSD, California San Diego
Bhupendra Goswami	MS12	Assistant Professor at Central University of Rajasthan
Ankit	MS12	PhD at IISER Mohali
Aleena Anna Thomas	MS12	PhD at IFW, Dresden, Germany
Mushir Ul Hassan	MS12	PhD at Temple University, USA
Anuj Pennathur	MS12	PhD at University of Southern California, USA
Anirudh CR	MS12	PhD at Michigan State University, USA
Mustafa Iqbal	MS12	PhD at TU Vienna, Austria
Ravi Ranjan	MS12	PhD at University of Illinois, Chicago, USA
Sruthy Chandy	MS12	PhD at Indiana University, Bloomington, USA
Ajit Kumar Yadav	MS12	Kota Institute Faculty
Siddhant V. Wagulde	MS12	PhD at University of Illinois, Chicago, USA
Vikram Singh Bhati	MS12	Kota Institute Faculty
Nimya SS	MS12	PhD at Indian Institute of Tropical Meteorology, Pune
Vikram Singh Bhati	MS12	ALLEN Career institute, Kota
Sumit Kumar Agarwal	MS12	PhD at BITS Pilani
Ebin George	MS12	Assistant Manager, SBI
Bharti Sohpal	MS12	Team Lead and SME- Chemistry, Evelyn Learning Systems Pvt. Ltd.
Shreyan Ganguly	MS13	PhD at IISER Mohali
Ankit Somani	MS13	Ph. D. at Ruhr University Bochum, Germany
Vaishnavi Sidharthan	MS13	Ph. D. at the Ohio State University, USA
Neelima PR	MS13	M. Phil. student at CUSAT Kochi, India
Chaman Lal Mahawar	MS13	Inspector, Central Board of Excise and Customs (CBEC), Kolkata
Saurabh Mhatre	MS13	PhD at FSU Jena, Germany
Anuj Kumar	MS13	PhD at TU, Delft, Netherlands
Meghanad Kayanattil	MS13	PhD at Max Planck Institute (Hamburg, Germany)
Pragya Verma	MS13	PhD at University of Geneva, Switzerland
Divita Gupta	MS13	PhD at Universite de Rennes, France
Priyanka Bansal	MS13	PhD at EPFL, Switzerland
Amala Raj	MS13	Ph. D. at Indiana University, USA

Alumni Placements

Chemistry major (MS) students

Name	Batch	Current Position
Omprakash	MS13	Faculty, Allen Institute, Chennai
Ajit Kumar Yadav	MS13	Faculty, Allen Institute, Chennai
Siddharth K Kurdia	MS13	MBA, IBS, Mumbai
Irin P Tom	MS14	PhD at University of Illinois at Chicago, USA
Amal Sam Sunny	MS14	PhD at University of Miami, USA
Vaitheesh J	MS14	PhD at University of Miami, USA
Virinder Bhagat	MS14	PhD at University of Tuebingen, Germany
Amandeep Singh	MS14	PhD at IISER Mohali
Divanshu Gupta	MS14	PhD at University of Tuebingen, Germany
Shiny Maity	MS14	PhD at University of California, Santa Barbara, USA
Priyasha Deshpande	MS14	PhD at CUNY, New York, USA
Nayana BC	MS14	PhD at Indiana University, USA
Mythreyi RM	MS14	PhD at University of Southern California, USA
Vishal Tiwari	MS14	PhD at University of Rochester, USA
Rishabh Gupta	MS14	PhD at Purdue University, USA
Shruthi S. Nair	MS14	PhD at Friedrich Schiller Universitat Jena, Germany
Suresh Kumar	MS14	PhD at Friedrich Schiller Universitat Jena, Germany
Leijish VP	MS14	PhD at University of Eastern Finland
Pinku Tung	MS14	PhD at University of Illinois, Chicago, USA
Shivangi Kharbanda	MS14	PhD at Oklahoma State University, OK, USA
Rishab Gupta	MS14	PhD at Purdue University, West Lafayette, USA
Abdul Haseeb MM	MS14	PhD at University of Illinois, Chicago, USA
Md Misbahur Rehman	MS14	PhD at King Abdullah University of Science and Technology, UAE
Vishal Porwal	MS14	PhD at University of Lorraine, France
Himanshi Singh	MS14	PhD at Deutsche Electron Synchrotron, Hamburg, Germany
Ajeet Kumar	MS14	PhD at Technical University of Munich, Germany
Kripa Joseph	MS14	PhD at University of Strasbourg, Strasbourg, France
Vidhya Lakshmi	MS14	PhD at The Ohio State University, USA
Jai Khatri	MS14	PhD at Ruhr University, Bochum, Germany
Diksha Sharma	MS14	MBA at XLRI, Jamshedpur, India
Parth Raval	MS14	PhD at University of Lille, France
Isabella Antony	MS14	Project assistant, IISER Mohali
Nihal PC	MS14	College Teacher
Manish Kumar Yadav	MS14	PhD at Ariel University, Israel
Nitish Kumar Garg	MS14	PhD at University of Lund, Sweden
Debanjan Chowdhury	MS15	PhD at Heidelberg University
Parmeet Kaur Dhindsa	MS15	PhD at Rice University
Anees Rahman P	MS15	Chemistry Faculty at DOPA-Doctors Own Preparation Academy
Anjana R Kammath	MS15	PhD at Yale University
Ashitha P P	MS15	PhD at Catalan Institute of Nanoscience and Nanotechnology (ICN2), Autonomous University of Barcelona
Sudha Yadav	MS15	PhD at Johns Hopkins University
Adarsh R	MS15	PhD at Syracuse University
Nahas K	MS15	Chemistry Faculty at Rays entrance coaching center
Preeti	MS15	System Operator at Regional Municipality of Niagara
Raj Kumar	MS15	PhD at Utrecht University
Vaibhav Pal	MS15	PhD at Penn State University
Harikrishnan R	MS15	PhD at University of Canterbury
Saurabh Nandkumar	MS15	MBA at IIM Calcutta

Alumni Placements

Chemistry major (MS) students

Name	Batch	Current Position
Lincoln	MS15	PhD at University of California San Diego
Ishan Sarkar	MS15	PhD at Chalmers University of Technology
Sahil Kaushal	MS15	PhD at IISER Mohali
Thabassum Ahammad Nk	MS15	PhD at University of Southern California
Dharm Singh Yadav	MS15	PhD at Universitatea de Medicină și Farmacie, Carol Davila” din București
Athul Vijay V C	MS15	PhD at University of Illinois, Chicago, USA
Arghadip Koner	MS15	PhD at University of California San Diego
Prashant	MS15	PhD at Eindhoven University of technology
Harpreet Kaur	MS15	PhD at University of Saskatchewan
Dhanvin M Koundinya	MS15	PhD at UiT, The Arctic University of Norway
Sandita Das	MS15	PhD at Iowa State University
Kale Milind Sanjay	MS15	PhD at CSIR- National Chemical Laboratory Pune
Chithra P.R	MS15	
Parkar Vidit Suryakant	MS15	
Megha	MS15	
Aakanksha Meena	MS15	
Shubham Ramle	MS15	
Sheetal Rani	MS15	
Sidharth Sh	MS15	
Lopamudra Das	MS15	
Rahul Singh Yadav	MS16	PhD in University of Zaragoza, Spain
Neha Bajaj	MS16	PhD at Ottawa University, Canada
Abhishek Kumar	MS16	MBA at IIM UDAIPUR
Shradha Sapru	MS16	PhD at Stanford University, USA
Reena	MS16	PhD at IISER Mohali
Ajay Jayachandran	MS16	PhD at the University of Würzburg, Germany
Vinod Gour	MS16	Research Assistant at IIT Ropar, India
Anuj Kaundal	MS16	MBA at IIT Bombay
Saumya Sebastian	MS16	PhD at Nanyang Technological University, Singapore
Ojas Singh	MS16	PhD at Maynooth University, Ireland
Divya Suman	MS16	PhD at EPFL, Switzerland
Kirti Devi	MS16	PhD at Ruhr University and Max-Planck-Institut für Kohlenforschung, Germany
Sparsh Tyagi	MS16	PhD at the University of Oxford, UK
Arjun Chowdhury	MS16	PhD at Boston College, USA
Deepraj Verma	MS16	PhD at Technion - Israel Institute of Technology, Israel
Yuvraj Vaishnav	MS16	PhD at Kaust University, Saudi Arabia
Hunarpreet Kaur	MS16	PhD at Radboud University, Netherlands
Harjasnoor Kakkar	MS16	PhD at the Autonomous University of Barcelona, Spain
Dhanyaj N. Nampoothiry	MS16	PhD at Indiana University, USA
Aljasil Chirakkal	MS16	PhD at University of Oslo, Norway
Adarsh S Kurup	MS16	PhD at University of Florida, USA
Rosmi Reji	MS16	PhD at University of Illinois, Chicago
Anshul Nagar	MS16	Lecturer at Allen Institute
Nikita Singh	MS16	
K Abhijeet	MS16	
Surajmal Nain	MS16	
Yashika Gupta	MS16	
Amisha Yadav	MS16	
Akhil Pratap	MS16	

Alumni Placements

Chemistry major (MS) students

Name	Batch	Current Position
Manisha Gaurav	MS16	
Salman Faris K	MS16	
Rajdeep Kiran	MS16	
Pravin Kumar	MS16	
Chetan	MS16	
Sajan Chinnan	MS16	
Rohit Kumar Naraniya	MS16	
Akhilesh Kumar Meena	MS16	
Umakant Gaurav	MS16	
Harsh Kishor	MS16	
Abhishek Dangi	MS16	
Sreelakshmi. V	MS16	
Pankaj Kumar Jangid	MS16	
Somesh	MS16	
Abhishek Roy	MS17	PhD at University of Rochester
Anwita Chattopadhyay	MS17	PhD at University of Rochester/ University of Texas at Dallas
Roshan Nasare	MS17	PhD at Tampere University
Praveen Bheraram	MS17	PhD at University of St Andrews
Abhinav Bansal	MS17	MBA, IIM Lucknow
Sahil Sharma	MS17	PhD at Purdue University
Vivek Yadav	MS17	PhD at Israel Institute of Technology, Haifa, Israel
Jaspreet Kaur	MS17	PhD at Brown University, US
Shounak Kishor Hinge	MS17	Scientific Researcher (University of Duisburg - Essen)
Prateek Pranjal	MS17	PhD at Autonomous University of Madrid
Vedang Abhijeet Puranik	MS17	PhD at Dartmouth College
Rajwant Kaur	MS17	MBA, IIM Ahmedabad
Harshit Jain	MS17	PhD at University of Illinois Urbana-Champaign
Parbhat Kumar	MS17	PhD at University of Rochester
Ankita Meena	MS17	Researcher, Polymer Institute of Slovak Academy of Sciences
Anish Kumar Singh	MS17	MBA, IIT Bombay
Omkar Charapale	MS17	PhD at Deakin University, Melbourne
Monu	MS17	
Amit Kumar	MS17	
Aman Jaiswal	MS17	
Sajal Nawaria	MS17	
Kavyasree A	MS17	
Hrishikesh K	MS17	
Divyanshu Baranwal	MS17	
Shambhu Prasad	MS17	
Nishant	MS17	
Kshitesh Lingala	MS17	
Ajay Jain	MS17	
Vishal Kataria	MS17	
Paras Yadav	MS17	
Malpath Kusha Sameeha	MS17	
Muhammed Anjad P P	MS17	
Yashoda Singh	MS17	
Tarunjeet Kumar	MS17	
Rupali Singh	MS17	
Ashwani Gurjar	MS17	

Alumni Placements

Chemistry major (MS) students

Name	Batch	Current Position
Shubham	MS17	
Aakanksha Kumari	MS17	
Yuvraj Yogesh	MS17	
Aditi Aggarwal	MS17	
Sneha Mehra	MS17	
Sachin Jadhav	MS17	
Aastha	MS18	PhD at Washington university in St Louis
Anshul	MS18	Placed in Dr. Reddy's Laboratory
Arkopal Nandy	MS18	PhD at Penn State University
Dheeraj Jangid	MS18	Preparing for Govt. Exam
Dhriti Maity	MS18	PhD at University of Rochester
Jyotiranjana Mohanta	MS18	PhD at Baylor University
Munnu Kumar	MS18	PhD at Temple University
Pradhyuman Meena	MS18	Preparing for Govt. Exam
Pratibha Jakhar	MS18	PhD at University of Stuttgart
Sagnik Chakraborty	MS18	PhD at St Louis University
Sankalp Agrawal	MS18	
Sameer Yadav	MS18	
Neeraj Pratap Singh	MS18	
Abhinandan Prakash	MS18	
Aman Kumar Sharma	MS18	
Ankit Phutela	MS18	
Arshdeep Singh Bains	MS18	
Atharva Jadhav	MS18	
Dheeraj Kumar Meena	MS18	
Harsh Vardhan Singh	MS18	
Harshita Sawdekar	MS18	
Jeevan Lakshmi Raj	MS18	
Saragadam	MS18	
Jyoti Swami	MS18	
Nitika	MS18	
Piyush Saini	MS18	
Pooja Dhayal	MS18	
Integrated PhD opted for MS degree		
Kaustav Chatterjee	MP15	PhD at Indiana University, USA
Pankaj Seliya	MP16	PhD at Max Planck Institute for Polymer Research, Germany
Soumyadeep Chakravarty	MP16	PhD at University of Rostock, Germany
Kausalandra Patel	MP16	PhD at IISER Mohali
Basundhara Dasgupta	MP18	PhD at University of Berlin

Alumni Placements

Former PhD students

Name	Year of passing	(supervisor) present position
Dr. Sadhika Kullar	2013	(Prof. Sanjay Mandal), Assistant Professor, NIT Jalandhar
Dr. Neha Jain (Bio PhD)	2013	(Prof. Samrat Mukhopadhyay), Assistant Professor, IIT Jodhpur
Dr. Zeba Qadri	2014	(Dr. Ramesh Ramachandran), Postdoc at Harvard Medical School, Boston
Dr. Shruti Arya	2015	(Prof. Samrat Mukhopadhyay) Postdoc at Univ. of California Santa Barbara, USA
Dr. Dominic Narang	2015	(Prof. Samrat Mukhopadhyay), Postdoc at University of California San Diego, USA
Dr. Vijit Dalal	2015	(Prof. Samrat Mukhopadhyay), Scientist, Benitec Inc. San Francisco Bay Area, USA
Dr. Gurpreet Kaur	2015	(Dr. Angshuman Roy Choudhury), Assistant Professor, DAV University, Jalandhar
Dr. Navnita Kumar	2015	(Prof. Sanjay Mandal), Postdoc: University of California, Los Angeles
Dr. Billa Prasanth	2015	(Prof. Sanjay Singh), Teaching at Narayana Institute, Hyderabad
Dr. R. Venkata S Rao	2016	(Dr. Ramesh Ramachandran), Postdoc at TCIS, Hyderabad
Dr. U. Sivarajan	2016	(Dr. Ramesh Ramachandran), Postdoc at Hebrew University
Dr. Seema Rani	2016	(Dr. S. S. V. Rama Sastry), Postdoc at the Technion, Israel
Dr. Nayyar A Aslam	2016	(Prof. S. A. Babu) Postdoc at UCSF, TCIP Hangzhou, Chinese Academy of Science
Dr. Kuldeep Jaiswal	2016	(Prof. Sanjay Singh) Postdoc at York University, Canada
Dr. Vadla Rajkumar	2016	(Prof. S. A. Babu), at GVK BioSciences, Hyderabad
Dr. C. Reddy	2016	(Prof. S. A. Babu) Postdoc with Dr. R. G. Bhat, IISER, Pune.
Dr. B. T. Ramanjaneyulu	2016	(Prof. R. Vijaya Anand), Postdoc at POSTECH, South Korea
Dr. Sumyra Sidiq	2016	(Prof. S. K. Pal) Assistant Professor, Govt degree college for women, University of Kashmir.
Dr. Shilpa Setia	2016	(Prof. S. K. Pal) Bhag Singh Khalsa College for Women, Abohor, Punjab
Dr. Naveen	2017	(Prof. S. A. Babu) Postdoc, Weizmann Institute of Science, Israel
Dr. R. Parella	2017	(Prof. S. A. Babu) Postdoc, University of Texas, USA
Dr. B. Gopalakrishnan	2017	(Prof. S. A. Babu) Postdoc, IIT Madras, India
Dr. Shruti Arya	2017	(Prof. Samrat Mukhopadhyay), Postdoc at University of California, Santa Barbara.
Dr. Hare Ram Yadav	2017	(Dr. Angshuman Roy Choudhury) Assistant Professor at the Department of Chemistry, Dr. B. R. Ambedkar Govt. Degree College, Maharajganj, UP under Siddharth University.
Dr. V. Venkat Reddy	2017	(Prof. R. Vijaya Anand), Postdoc at the University of Cape Town, SA
Dr. Panjab B. Arde	2017	(Prof. R. Vijaya Anand), Sailifesciences, Pune
Dr. Deependra Bawari	2017	(Prof. Sanjay Singh) Postdoc at Tel Aviv University
Dr. Mahesh Sriram	2017	(Prof. R. Vijaya Anand) Postdoc at the University of Auburn, USA
Dr. Monika Gupta	2018	(Prof. S. K. Pal) Ramanujan Fellow, Indian Institute of Technology, Ropar.
Dr. Abhijeet S. Jadhav	2018	(Prof. R. Vijaya Anand) Scientist at Jubilant Chemsys Ltd, Noida
Dr. Prithwish Goswami	2018	(Prof. R. Vijaya Anand) Scientist at Jubilant Chemsys Ltd, Noida
Dr. Moumita Rana	2018	(Dr. Ujjal K. Gautam) Postdoc at IMDEA Materials Institute, Madrid
Dr. Karishma Bhasne	2018	(Prof. Samrat Mukhopadhyay), Postdoc at University of Massachusetts, USA
Dr. Sudha Devi	2018	(Dr. Sugumar Venkataramani) College Lecturer.
Dr. Deependra Bawari	2018	(Prof. Sanjay Singh) Postdoc at UMR-CNRS at Toulouse, France
Dr. Ginny Karir	2018	(Prof. K. S. Viswanathan), Postdoc at IISc, Bangalore
Dr. Kanupriya Verma	2018	(Prof. K. S. Viswanathan), Postdoc at Purdue University, USA
Dr. Vinay Ganapathy	2019	(Dr. Ramesh Ramachandran), Postdoc at TCIS, Hyderabad
Dr. Bishnupada Satpathi	2019	(Dr. S. S. V. Rama Sastry) Postdoc, Weizmann Institute of Science, Israel (to be joined)
Dr. Narendra Bisht	2019	(Prof. S. A. Babu) Scientist at Jubilant Chemsys Ltd, Noida

Alumni Placements

Former PhD students		
Name	Year of passing	(supervisor) present position
Dr. Gayathri S. Singaraju	2019	(Dr. Sabyasachi Rakshit) Postdoc at IST Austria
Dr. Satyam Ravi	2019	(Dr. K. R. Shamasundar) Assistant Professor, VIT Bhopal
Dr. Anita Devi	2020	(Dr. Arijit K. De) Postdoc at the University of Alberta, Canada (Michael Woodside Group)
Dr. Sanjit Mandal	2021	(Dr. Ujjal K. Gautam) Postdoc at Ben Gurion University, Israel
Dr. Lipipuspa Sahoo	2021	(Dr. Ujjal K. Gautam) Postdoc at INST Mohali
Dr. Jagadish Prasad	2021	(Dr. Sabyasachi Rakshit) Postdoc at Oxford University, UK
Dr. Joydip De	2021	(Prof. S. K. Pal) Marie-Curie (MSCA) Fellow, University of St Andrews, UK
Dr. Indu Bala	2021	(Prof. S. K. Pal) Assistant Professor at IIT Mandi
Dr. Yogita Silori	2021	(Dr. Arijit K. De) Postdoc at University of Michigan, USA (Ogilvie Group)
Dr. Amreen K Bains	2022	(Dr. Debashis Adhikari) Postdoc at Colorado State University
Dr. Kirti Singh	2022	(Dr. Debashis Adhikari) Postdoc at University of California, Davis
Dr. Mayank Joshi	2022	(Dr. Angshuman Roy Choudhury) Assistant professor at AMITY University, Mohali, Punjab.
Dr. Jyoti Lather	2022	(Dr. Jino George) Postdoc at AMOLF, Amsterdam
Dr. Vidhika Punjani	2022	(Prof. S. K. Pal) Postdoc at the Centre of Molecular and Macromolecular Studies of the Polish Academy of Sciences (CMMS-PAS), Lodz, Poland
Dr. Shaina Dhamija	2022	(Dr. Arijit K. De) Postdoc at Max Planck Institute, Germany (Mischa Bonn Group)
Dr. Surbhi Grewal	2022	(Dr. Sugumar Venkataramani) Postdoc at Masaryk University (MUNI), Czech Republic
Dr. Sandeep K Thakur	2023	(Prof. Sanjay Singh) Postdoc at Friedrich Alexander University Erlangen-Nuremberg, Germany
Dr. Gurdeep Singh	2023	(Prof. R. Vijaya Anand) Postdoc at RWTH Aachen University, Germany
Dr. Samita Mishra	2023	(Dr. Arijit K. De) Postdoc at Bar-Ilan University, Ramat Gan, Israel (Yaakov Tischler Group)
Dr. Sonam Sharma	2023	(Prof. R. Vijaya Anand) Postdoc at the University of Regensburg, Germany
Dr. Ipsita Pani	2023	(Prof. S. K. Pal) Postdoc at the University of Munster, Germany
Dr. Kavita Rani	2023	(Dr. Sanchita Sengupta) Postdoc at University of Oxford, UK (Guide: Prof. H. L. Anderson)
Dr. Ekta Shandilya	2023	(Dr. Subhabrata Maiti) Postdoc at Pennsylvania State University, USA (joining soon)
Dr. Akshi Deshwal	2023	(Dr. Subhabrata Maiti) Assistant Professor, Punjab Engineering College, Chandigarh
Dr. Pooja Bhatt	2023	(Dr. Jino George) Postdoc at Tel Aviv University, Israel
Dr. Surbhi Garg	2023	(Dr. Sabyasachi Rakshit) Postdoc at Emory University
Dr. Mamta Bhandari	2023	(Prof. Sanjay Singh) Postdoc at Rice University, USA.

Awards and Recognitions

Faculty

- ❖ Ujjal Gautam has been selected for the MRSI (Materials Research Society of India) Medal for 2023.
- ❖ Kuduva R. Vignesh has received the Start-up research grant from SERB in 2023 (Grant no. SRG/2023/000286)
- ❖ Suman K. Barman has received the DST-SERB-EEQ grant (EEQ/2022/000786) in 2023.
- ❖ S. A. Babu has been selected as one of the recipients of the CRSI Bronze Medal 2023.
- ❖ Subhabrata Maiti has been chosen as an Editorial Advisory Board member of ChemSystemsChem (2023)
- ❖ Debashis Adhikari has joined Organometallics (ACS) as a guest editor for the forum in Photocatalysis.
- ❖ Sanchita Sengupta has received the ministry of education (MoE)-STARS research grant in 2023.
- ❖ Ujjal K Gautam has received the Chemical Research Society of India (CRSI) Bronze Medal. (2023)
- ❖ Sugumar Venkataramani has received the Chemical Research Society of India (CRSI) Bronze Medal. (2023)
- ❖ Samrat Mukhopadhyay has been elected as a Fellow of the Indian Academy of Sciences (2023).
- ❖ Samrat Mukhopadhyay has been appointed as Chair-Elect, Intrinsically Disordered Proteins subgroup of the Biophysical Society (USA).
- ❖ Samrat Mukhopadhyay has become a Council Member of the Indian Biophysical Society
- ❖ Samrat Mukhopadhyay has been appointed as program co-chair of the Intrinsically Disordered Protein (IDP) subgroup symposium of the Biophysical Society meeting that will be held in February 2023 in San Diego, USA.
- ❖ Sanjay Singh has joined the advisory board of the journal ChemistrySelect (Wiley) (2022-2026).
- ❖ Sanchita Sengupta has received the Chemical Research Society of India (CRSI) Young Scientist Award (2022).
- ❖ Sanchita Sengupta has been appointed as an early career advisory board (ECAB) member of the journal ChemistrySelect (Wiley) (2022).
- ❖ Sanchita Sengupta has received the Science and Engineering Board (SERB) POWER research grant in 2022 (Grant no. SPG/003570).
- ❖ Arijit Kumar De has received the Core-research grant from SERB/DST for three years (CRG/2021/003981).
- ❖ Arijit Kumar De has received International Travel Support from INSA, India: 06/06/2022. (INSA travel grant No. SS/INSA/2022/60)
- ❖ Arijit Kumar De has received the Presider of the Session on "Dynamics of Complex Systems" at the International Conference on Ultrafast Phenomena-2022; Montréal, Quebec, Canada; 18-22 July, 2022.
- ❖ Santanu Kumar Pal is a recipient of the prestigious CRS Silver Medal (2022) for his academic achievement.
- ❖ Santanu Kumar Pal became a fellow of the Royal Society of Chemistry (FRSC), UK, in 2022.
- ❖ R. Vijaya Anand has received the Chemical Research Society of India (CRSI) Bronze Medal (2022).
- ❖ S. S. V. Ramasastry selected to receive the prestigious CDRI Award for Excellence in Drug Research 2022
- ❖ S. S. V. Ramasastry has joined the Editorial Board of the RSC journal "Organic & Biomolecular Chemistry"
- ❖ Jino George has received the Young Scientists Award 2021- Asian Oceanian Photochemistry Association, APA (JAPAN) for "Controlling Chemical and Physical Properties of Molecules by Light-Matter Strong Coupling"
- ❖ Debashis Adhikari has received DST-Core-research grant in 2021 (DST-CRG-001951)
- ❖ Suman K. Barman has received the SERB Start-up research grant (SRG/2021100 1570) in 2021.
- ❖ Suman K. Barman has received DST-Inspire Faculty Research grant (DST/INSPIRE/04/2020/002347) in 2021
- ❖ Subhabrata Maiti has been elected as Review Editor for Frontiers in Chemistry | Supramolecular Chemistry
- ❖ Sabyasachi Rakshit has been invited to serve as Guest Editor for Frontiers in Molecular Biosciences.
- ❖ Sabyasachi Rakshit has become a member of the Early Career Taskforce for Portland Press, UK.
- ❖ S. V. Rama Sastry Sripada has received the RSC Research Fund grant. (2020)
- ❖ Debashis Adhikari has joined the editorial advisory board of Chemistry Open (2020)
- ❖ R Vijaya Anand has been appointed to the editorial board of Resonance.
- ❖ Santanu K Pal has received the Chemical Research Society of India (CRSI) Bronze Medal. (2020)
- ❖ Subhabrata Maiti has received SERB-Early Career Research Award (2020)
- ❖ Sugumar Venkataramani has received Indo-Czech Republic Cooperative Scientific Research grant sponsored by DST.
- ❖ Subhabrata Maiti (PI) and Dr. Santanu K. Pal (Co-PI) have received MHRD-STARS grant in 2020.
- ❖ Jino George (PI) has received MHRD-STARS grant in 2020
- ❖ Samrat Mukhopadhyay has been appointed to the Editorial Board of the Biophysical Journal (Cell Press) (2020).
- ❖ Samrat Mukhopadhyay has been appointed to the Editorial Advisory Board, Journal of Physical Chemistry (2019-2021)
- ❖ Samrat Mukhopadhyay has been appointed to the Editorial Board of Essays in Biochemistry (Biochemical Society, London) (2019).

Awards and Recognitions

Faculty

- ❖ Samrat Mukhopadhyay has been appointed as an Editorial Board Member, Journal of Cellular Biochemistry (Wiley) (2020-)
- ❖ Samrat Mukhopadhyay has been appointed as the Ambassador of the Biophysical Society (USA) (2019).
- ❖ Samrat Mukhopadhyay has been invited to write a Feature Article in the Journal of Physical Chemistry (American Chemical Society) (2019).
- ❖ Samrat Mukhopadhyay has received the Bronze Medal from the Chemical Research Society of India (CRSI) 2019
- ❖ Monika Sharma has received the Bharat Vikas Award for the year 2019.
- ❖ Debrina Jana has been selected as community board member in "Nanoscale Horizons" by the Royal Society of Chemistry (2019).
- ❖ Raj Kumar Roy has received SERB-Early Career Research Award (2018)
- ❖ S. S. V. Ramasastry was awarded Swarnajayanti Fellowship, from the Department of Science & Technology (DST), Govt. of India (2017-2018).
- ❖ S. S. V. Ramasastry has received Young Scientist Award from A. V. Rama Rao Research Foundation (AVRA) (2018).
- ❖ S. S. V. Ramasastry has received Organization of Pharmaceutical Producers of India (OPPI) Young Scientist award. (2018)
- ❖ S. S. V. Ramasastry has received the Chemical Research Society of India (CRSI) Bronze Medal. (2018)
- ❖ S. S. V. Ramasastry has received Thieme Chemistry Journal's Award 2017 [Chosen by the Editorial Boards of Synlett, Synthesis, and Synfacts]
- ❖ S. S. V. Ramasastry has been chosen as an Editorial Advisory Board member of *Organic & Biomolecular Chemistry* (2017)
- ❖ P. Balanarayan received the best teacher's award from IISER Mohali (2017)
- ❖ Prof. N. Sathyamurthy has been elected the president of the Chemical Research Society of India (CRSI) for a period of three years from April 01, 2017.
- ❖ Debashis Adhikari has received SERB-Early Career Research Award (2018)
- ❖ Arijit Kumar De has received DST travel fellowship to attend Gordon Conference on "Quantum Control of Light and Matter", USA, 2017. (Application No. - ITS/Off-502/2017-18)
- ❖ Arijit Kumar De has received INSA travel fellowship to attend Gordon Conference on "Quantum Control of Light and Matter", USA, 2017. (INSA travel Grant No. SS/INSA/2017/758)
- ❖ Arijit Kumar De has received SERB, DST Early Career Research Award, 2016. (Grant No: ECR/2016/000467)
- ❖ S. S. V. Ramasastry has received the young scientist award from the organizing committee of 'Chemical Frontiers-2016
- ❖ S. S. V. Ramasastry has been admitted as a Member of the Royal Society of Chemistry (MRSC) in 2016
- ❖ Sabyasachi Rakshit has received Welcome Trust/DBT Intermediate Fellowship, DBT. (2015-2020)
- ❖ Santanu Kumar Pal has received INSA medal for Young Scientist (2015)
- ❖ Samrat Mukhopadhyay has received Commonwealth Science Follow-on Grant from the Royal Society London (2015)
- ❖ Santanu Kumar Pal has received NASI-Young Scientist platinum Jubilee award (2015)
- ❖ Santanu Kumar Pal has received International Travel award from DST-SERB to attend in Optics of liquid crystals conference held in Sopot, Poland. (2015)
- ❖ Samrat Mukhopadhyay has received the International Travel Award from the Immunology Foundation to attend the Protein Society meeting held in San Diego, California, USA. (2014)
- ❖ Samrat Mukhopadhyay has received the Prof. B.K. Bachhawat International Travel Award for Young Scientists to attend the Biophysical Society meeting held in San Francisco, California, USA. (2014)
- ❖ Santanu Kumar Pal has received Young Achiever Award from DAE-BRNS (2014)
- ❖ Ramesh Ramchandran received the best teacher's award from IISER Mohali (2013)
- ❖ Santanu Kumar Pal has received DAE Young Scientist Research Award (2012)
- ❖ Sanjay Singh was elected as Young Associate of the Indian Academy of Sciences in Bangalore (2009-2013)
- ❖ Samrat Mukhopadhyay has been selected as a Young Associate of the Indian Academy of Sciences. (2009-2013)
- ❖ Samrat Mukhopadhyay has been invited to contribute profile annual issue of 'Who's who in Fluorescence' (Published by Springer. Editor: Chris D. Geddes, University of Maryland Baltimore County). (2009)

Awards and Recognitions

Students, Postdocs and Research Associates

- ❖ Surbhi Bansal (PhD Student/Prof. SS Group) received the third prize for poster presentation in CHASCON-2-23, National Conference on Global Science for Global Wellbeing during October 12-14, 2023 at Punjab University.
- ❖ Ayanagshu Biswas (PhD Student/Dr. DA Group) received the third prize for poster presentation in CHASCON-2-23, National Conference on Global Science for Global Wellbeing, October 12-14, 2023 at Punjab University.
- ❖ Ritobrata De (PhD student/Prof. SKP group) received the Best Oral Presentation Award at the "5th International Conference on Advanced Materials for Better Tomorrow-II (AMBT) 2023" conducted by the Society or Interdisciplinary Research in Materials and Biology (SIRMB) and hosted by the Department of Physics, Banaras Hindu University between October 10-13, 2023.
- ❖ Subho Mitra (PhD student/Dr. AKDe group) received two prestigious awards (Carl Storm International Diversity (CSID) Fellowship from GRC (complete waiver of Registration fees) and Researcher Development and Travel Grant of £500 from the Royal Society of Chemistry (for travel) in addition to travel support from SERB to attend the 2023 Quantum Control of Light and Matter Gordon Research Conference held at Salve Regina University (USA) from 6 to 11, August 2023.
- ❖ Maqsuma Banoo (PhD Student/Dr. UKG Group): Best poster award in Indo-French Workshop on Clean and Sustainable Energy Technologies (INFINITE), 21-24 February, 2023.
- ❖ Shallu Dhingra got the International Liquid Crystal Society Student Travel Fund 2023 to attend the 2023 Gordon research conference in Liquid Crystal.
- ❖ Gayathri Parthiban (Dr. SV group): Best poster award at the RABMC-2022 (Recent Advances in Bioorganic and Medicinal Chemistry) Symposium Organized by NIPER S.A.S Nagar on November on 19th November, 2022.
- ❖ Shruti Rani received the best poster award at an International Conference on emerging materials for sustainable development in 2022.
- ❖ Maqsuma Banoo (PhD Student/Dr. UKG Group): Best Poster award at International Conference on Emerging Materials for Sustainable Development (EMSD-2022) held at CRSI-CSIO Chandigarh, 9-11th July 2022.
- ❖ Maqsuma Banoo (PhD Student/Dr. UKG Group): Best poster award in 29th CRSI-ACS symposium in chemistry held at IISER Mohali, 7-9 July 2022.
- ❖ Ritobrata De received the best poster at the 29th CRSI-NSC, organized by IISER Mohali in July 2022.
- ❖ Raj Sekhar Roy (PhD Student/Dr. UKG Group): Best oral presentation at International Conference on Emerging Materials for Sustainable Development (EMSD-2022) held at CRSI-CSIO Chandigarh, 9- 11 July 2022.
- ❖ Raj Sekhar Roy (PhD Student/Dr. UKG Group): Best poster award at International Conference on Engineering Trends in Science and Technology (ICETST), 10-11 June 2022
- ❖ Sumit Yadav. "Student Conference Support" travel grant from SPIE for attending "SPIE Photonics West 2022" (Not availed).
- ❖ Shaina Dhamija, ACS Journal of Physical Chemistry Award for her poster at the 29th CRSI-NSC conference 2022.
- ❖ Ankit Kumar Gaur (Dr. SV group): Best poster award at the International Symposium on Recent Advances in self-assembled Materials a Supramolecular Chemistry Organized by GNDU on 19th March 2022.
- ❖ Ramandeep Kaur (PhD student/Dr. S A Babu): received the best oral presentation award in the 29th CRSI-NSC symposium organized at IISER Mohali.
- ❖ Surbhi Garg (PhD student/Dr. Sabyasachi Rakshit): awarded a travel grant from the International Union of Biochemistry and Molecular Biology (IUBMB) for attending "The Biochemistry Global Summit, Lisbon" organized by IUBMB-FEBS-PABMB Congress.
- ❖ Nisha Arora (PhD student/Dr. Sabyasachi Rakshit): awarded a travel grant from the International Union of Biochemistry and Molecular Biology (IUBMB) for attending "The Biochemistry Global Summit, Lisbon" organized by IUBMB-FEBS-PABMB Congress.
- ❖ Jay Prakash (PhD student/Dr. SSVR group): won the best oral presentation award at the International Conference on 'Emerging Trends in Science and Technology', organized by the Punjab Engineering College (PEC) Chandigarh on 10 and 11-June, 2022.
- ❖ Mr. Subhendu Samanta (PhD student/Dr. RKR group): Best Poster Award by ACS in the National Conference May 2022 on Polymer Science and Technology organized by SPSI Mumbai Chapter.
- ❖ Mr. Subhendu Samanta (PhD student of Dr. Raj Kumar Roy): Best Poster Award by ACS in the CRSI-NSC 2022 organized by IISER Mohali.
- ❖ Debapriya Gupta received a SERB-ITS Travel Grant (ITS/2022/000969) for attending the 28th PhotoIUPAC in Amsterdam, Netherlands.

Awards and Recognitions

Students, Postdocs and Research Associates

- ❖ Debapriya Gupta received an RSC Researcher Development Grant for attending the 28th Photo IUPAC in Amsterdam, Netherlands.
- ❖ Sakshi Chawla, Honorable Mention Award at Ultrafast Sciences (UFS 2022), IISER Thiruvananthapuram
- ❖ Abdul Alim, Best Poster Award at the XLV Symposium of the Optical Society of India Conference on Optics, Photonics & Quantum Optics (COPaQ 2022), IIT Roorkee, India.
- ❖ Shaina Dhamija, Best Thesis Award at the XLV Symposium of the Optical Society of India Conference on Optics, Photonics & Quantum Optics (COPaQ 2022), IIT Roorkee, India.
- ❖ Shaina Dhamija, Best Oral Presentation Award at the IX International Conference on Perspective in Vibrational Spectroscopy (ICOPVS-2022), Indore, India.
- ❖ Subhash Chander was selected to participate in the 10th Research Opportunities Week (ROW) at the Technical University of Munich (TUM), Germany (2022).
- ❖ Mamta Bhandari: Best poster award in an International Conference Main Group Molecules to Materials (MMM-II) organized by NISER Bhubaneswar in December 2021
- ❖ Amreen K Bains (PhD student/ DA lab) became a recipient of J-NOST student award (2021)
- ❖ Amreen K Bains (PhD student/ DA lab) became a recipient of KVR Rao fellowship award (2021)
- ❖ Akhila Kadyan (Molecular Strong Coupling Group): Best prize for the poster presented in the Spectroscopy session (ACS Physical Chemistry Au) of the 27th CRSI National Symposium in Chemistry 2021.
- ❖ Sakshi Chawla (PhD), ACS Applied Energy Materials Award at CRSI-NSC 26 Award for her poster entitled "Unravelling the role of water in ultrafast excitation energy transfer within nano- architectures of chlorophyll ".
- ❖ Samita Mishra (PhD), ACS Omega Award at CRSI-NSC 26 for her poster entitled "Charge transfer dynamics and stability enhancement in inorganic halide perovskite solar cells"
- ❖ Shradha Sapru (MS). Best academic performance in class of 2021.
- ❖ Shradha Sapru (MS). Excellence award in Chemistry 2021.
- ❖ Shaina Dhamija. "FiO + LS Incubic Milton Chang" travel grant from Optical Society of America (OSA) for attending "Frontiers in Optics/Laser Science" Conference.
- ❖ Anita Yadav. Fullbright Nehru Post Doctoral Fellowship by United States-India Educational Foundation (USIEF).
- ❖ Shaina Dhamija, International Travel Support (ITS), Science and Engineering Research Board, DST, India (Travel grant no. ITS/2021/000272)
- ❖ Shaina Dhamija, International Travel Grant, Council of Scientific & Industrial Research, DST, India (Travel grant no. TG/11385/21-HRD) (Not availed).
- ❖ Subhash Chander, DSK Postdoctoral Fellowship by the UGC, New Delhi. June 23, 2020.
- ❖ Sumit Yadav, International Travel Support (ITS), Science and Engineering Research Board, DST, India (Travel grant no. ITS/2021/000218) (Not availed).
- ❖ Jagadish P. Hazra: Received Scirox award (Cash prize and Citation) for Science Outreach from Punjab Soc. For Promotion of Science Technology and Innovation and Guru Nanak Dev University 2021.
- ❖ Nisha Arora: Selected for online research presentation on MechanoChemBio2021 organized by Max Planck Institute of Colloids and Interfaces, MPI 2021.
- ❖ Subhash Chander, ACS Bridge Fellow by the American Chemical Society (ACS). October 27, 2020.
- ❖ Sumit Yadav, International Travel Grant, Council of Scientific & Industrial Research, India (Travel grant no TG/11374/21-HRD) (Not availed).
- ❖ Ekta Shandilya: Best poster award in CRIKC conference in chemistry held at IISER Mohali, November 2019.
- ❖ Anita Devi, travel grant from DST, India (Travel grant No.ITS/2019/001688).
- ❖ Subhash Chander, was selected as a member of 2019 CAS Future Leader by CAS.
- ❖ Yogita Silori, travel grant from International Travel Support (ITS), Science and Engineering Research Board, DST, India (Travel grant No. ITS/2019/002654).
- ❖ Mayank Saraswat (MP13): CSIR travel grant for attending International Symposium on Molecular Spectroscopy (ISMS), University of Illinois, Urbana-Champaign, USA.
- ❖ Gayathri S Singaraju: Travel grant for EMBO EMBL Symposium: "Mechanical Forces in Development" in July 2019 organised at EMBL Heidelberg, Germany.
- ❖ Gayathri S Singaraju: Research excellence award in 12th EBSA | 10th ICBP-IUPAP Congress, Madrid, Spain, July 2019.
- ❖ Jagadish P Hazra: Travel grant from the International Biophysical Society to deliver a talk at the annual meeting of the Biophysical Society meeting held in Baltimore, USA, 2019.

Awards and Recognitions

Students, Postdocs and Research Associates

- ❖ Sanjit Mondal (PH15009) First Indian, best poster award, Materials Conclave and the 30th Annual General Meeting of MRSI, 2019, Bangalore, India
- ❖ Ms. Jyoti Lather (PH17015): Best poster award, CRSI 2019
- ❖ Lipipuspa Sahoo (PH15057) best poster award, RAOBC 2019, Mohali, India
- ❖ Subhash Chander received 2019 CAS Future Leaders Award by the ACS Publications.
- ❖ Rajib Kr Nandi, received best Poster Award in NPDF online poster competition 2017-18, jointly organized by American Chemical Society via ACS Publications and Science and Engineering Research Board (SERB), India. The award ceremony "1st Conclave of SERB NPDF Awardees" was held at NIPGR, New Delhi on July 25, 2018.
- ❖ Jagadish P Hazra: Best poster award in ACS on campus (2018)
- ❖ Jagadish P Hazra: Best poster award in FCS 2018, at JNU, New Delhi.
- ❖ Ankit Somani (MS13): Best poster award inter IISER NISER chemistry meet, Dec 2017
- ❖ Bishnupada Sathpathi received the BEST poster award from the organizers of the 'Thematic Conference in Chemical Sciences (TC2S-2017): Sustainable Chemistry' held at IIT Ropar during May 15-16, 2017.
- ❖ Deependra Bawari (PhD student/SS group) received International Travel award from DST-SERB to attend the 12th International Symposium on Macrocyclic and Supramolecular Chemistry, 02-06 July, 2017 (Cambridge, London (UK).
- ❖ Jagadish P Hazra: Best poster award in Indian Biophysical Society meet, 2017.
- ❖ Deependra Bawari (PH12113), Best poster award in MTIC-XVII, 2017 at NCL Pune & IISER Pune.
- ❖ Deependra Bawari (PH12113) Recipient of International Travel Support: SERB, New Delhi to participate in the 12th International Symposium on Macrocyclic and Supramolecular Chemistry, Cambridge (UK): July 2017.
- ❖ Deependra Bawari (PhD student/SS group) attended the 11th International Symposium on Macrocyclic and Supramolecular Chemistry, 10-14 July, 2016. Travel support by IISER Mohali
- ❖ Seema Dhiman received the Eli-Lilly Outstanding Thesis Award 2016.
- ❖ Gayathri S Singaraju: Received Best Poster in 'Optics Within Life Sciences (OWLS) 2016' organized at TIFR, Mumbai,
- ❖ Anamika Mukhopadhyay (Postdoc/Prof. K. S. Viswanathan's group) has received CSIR Pool Scientist award. (2015)
- ❖ Indu Verma (PhD Student/SK Pal Group) won The Dewan Jawahar Lal Nayar Memorial prize at the 21st National Conference on Liquid Crystals (NCLC) held at VSSD College, CSJM University, Kanpur, and received best poster award. (2014)
- ❖ Sumyra Sidiq (PhD Student/SK Pal Group) has received International Travel award from DST-SERB to attend International Liquid crystal conference (ILCC) held in Trinity college, Dublin, Ireland. (2014)
- ❖ Gurpreet Kaur (Graduate student/ARC group) received the best oral presentation award in the 42nd National Seminar on Crystallography held in JNU, New Delhi. (2013)
- ❖ Sadhika Khullar (Graduate student) has defended her thesis entitled "Metal-Organic Coordination Networks Comprised of Divalent Metal Centers and Multiatom Carboxylate Linkers" under the supervision of Dr. Sanjay Mandal and graduated as a first doctoral student from the department. (2013)
- ❖ Shilpa Setia (Graduate student/SKPal group) won The Dewan Jawahar Lal Nayar Memorial prize at the 20th National Conference on Liquid Crystals (NCLC) (best poster presentation). (2013)
- ❖ Sumyra Sidiq (Graduate student/SKP group) has been adjudged the best in poster presentation and won The Dewan Jawahar Lal Nayar Memorial prize at the 19th NCLC held at the Thapar University, Patiala. (2012)
- ❖ Gurpreet Kaur (Graduate student/ARC group) has received Best poster award in 20th International Conference on the Chemistry of Organic Solid State held in IISc Bangalore. (2010)

Awards and Recognitions

The following BS-MS students received fellowships for summer internship abroad and other institutes within India.

S. No.	Name of the student/Batch	Place of visit	Year	Fellowship
1.	Kapil Dave/MS08	Ruhr University, Bochum, Germany	2012	DAAD-WISE fellowship
2.	Manish Pareek/MS08	University of Münster, Germany	2012	DAAD-WISE fellowship
3	Asif Equbal/MS08	ETH Zurich, Switzerland	2012	Summer internship
4	Gaurav Kumar/MS08	IST Austria	2012	Summer internship
5	Agastya P. Bhati/MS09	Freie Universitat, Berlin, Germany	2012	DAAD-WISE Young Ambassador
6	Agastya P. Bhati/MS09	University of Coimbra, Portugal	2013	Summer internship
7	Deepak Verma/MS09	St. Andrews University, Scotland	2013	Summer internship
8	Gargi Satish Jagdale/MS10	Taiwan	2014	Winter internship for two weeks
9	Rupali Chawla/MS10	Freie Universitat Berlin, Germany	2014	Inspire-FU Summer
10	Shwetha Srinivasan/MS11	Max Planck Institute of Biophysics, Germany	2014	Post Lindau Fellowship
11	Shwetha Srinivasan/MS11	University of Leipzig, Germany	2015	DFG for stay and subsistence in Germany, INSPIRE travel grant for travel
12	Srijit Mukherjee/MS11	University of Heidelberg, Germany	2015	DAAD-WISE fellowship
13	Aayush/MS12	University of Münster, Germany	2015	DAAD-WISE fellowship
14	Divita Gupta/MS13	Physical Research Laboratory, Ahmedabad, India	2016	Summer Internship
15	Rishabh Gupta/MS14	BARC, Mumbai	2016	Indian academy of sciences (IAS)
16	Anjana/MS15	CUSAT, Cochin	2016	VSRP fellowship
17	Priyanka Bansal/MS13	Indiana University, USA	2017	Summer Internship
18	Divita Gupta/MS13	University of Rennes 1, France	2017	Summer Internship
19	Rishabh Gupta/MS14	TIFR Hyderabad	2017	VSRP fellowship
20	Himanshi Singh/MS14	IISER, Pune	2017	SSPC fellowship
21	Vidhyalakshmi.S/MS14	TIFR, Hyderabad	2017	VSRP fellowship
22	Parth Raval /MS14	BARC, Mumbai	2017	Institute fellowship
23	Anjana/MS15	TIFR TCIS Summer Res. Hyderabad	2017	VSRP Fellowship
24	Vaibhav Pal/MS15	Centre for Nano and Soft Matter Sciences (CeNS), Bengaluru	2017	ROIS
25	Anjana Kammath/MS15	University of Chicago	2018	S N Bose Fellowship
26	Anjana Kammath/MS15	MPI MCBG, Germany	2019	DAAD Fellowship
27	Sudha Yadav/MS15	University of Rochester	2019	USA summer program
28	Arjun Chowdhury/MS16	IISER Bhopal	2019	Inspire
29	Rosmi Reji/MS16	IISc Bangalore	2019	IPC-SRFP 2019
30	Kirti Devi/MS16	IIT Bombay	2019	No Fellowship
31	Adarsh S Kurup/MS16	NIIST- CSIR, Thiruvananthapuram	2019	Inspire
32	A. Jayachandran/MS16	IISc Bangalore	2019	Inspire
33	Salman Faeris K/MS16	Calicut university	2019	Calicut University
34	Divya Suman/MS16	TIFR, Mumbai	2019	TIFR, Mumbai
35	Shradha Sapru/MS16	LMU-Munich	2019	DAAD-WISE
36	Sparsh Tyagi/MS16	Waterloo University	2019	Mitacs
37	Nikita Singh/MS16	Panjab University	2019	Inspire
38	Sreelakshmi V/MS16	RRI Bangalore	2019	Visiting students' program
39	Sajan Chinnan/MS16	Nagasaki University	2019	Inspire
40	Mohit Jaiswal/MS19	Israel Institute of Technology	2022	
41	Mohit Jaiswal/MS19	University of Basil	2023	

Curie Club

Curie Club, the chemistry club at IISER Mohali, run by chemistry major students, aims at inculcating scientific interest among the student community. The informal meetings of some chemistry enthusiasts every Saturday to discuss the advancements in Chemistry eventually gave rise to a now well-established student-run club. The club was christened the 'Curie Club' as its year of formation (2011) coincided with a century since Marie Curie was awarded the Nobel Prize in Chemistry for her seminal contributions to the field of radioactivity and which year was also declared as the International Year of Chemistry by IUPAC.



M. Curie

The club has active participation from undergraduates, graduates, and faculty. The activities organized by the club are scientific talks, both by speakers within IISER and other institutions. Students are encouraged to talk about their project work, demonstrate novel experiments, and disseminate their knowledge during outreach programs. Curie Club has also been organizing industrial visits to provide exposure to students for the applications of Chemistry in the industry.

Curie Club also celebrates a week-long event called "Curie Week". The events during the week include talks and interactive sessions by eminent scientists, activities such as descriptive writing, Quizzes, 'Ionic Soduku, Taboo, poster presentations, model making and sketching, and the much-enjoyed flagship event-Treasure hunt.

The club intends to reach a large section of the scientific community and showcase the cutting-edge chemistry research being conducted in IISER Mohali through outreach programs in schools and use social media to encourage students in the pursuit of science.



Members of the Curie Club demonstrated Chemistry experiments during the 17th Foundation Day of IISER Mohali.



The People

MS08 batch students



MS09 batch students



The People

**MS10 and Integrated
PhD 2012 batch
students**



**MS11 and Integrated
PhD 2013 batch
students**



**MS12 and Integrated
PhD 2014 batch
students**



The People

**MS13 and Integrated
PhD 2015 batch
students**



**MS14 and Integrated
PhD 2016 batch
students**



**MS15 and Integrated
PhD 2017 batch
students**



The People

**MS16 and Integrated
PhD 2018 batch
students**



**MS17 and Integrated
PhD 2019 batch
students**



MS17 batch students



The People

MS18 batch students



MS19 batch students



MS20 batch students



The People

MS21 batch students



PhD students



Integrated PhD students



The People

Postdoctoral fellows



Students group photo



Staff members



First row, (L to R): Mr. Triveni Shanker, Mr. Mangat Ram, Ms. Deepika, Ms. Reetu Chaudhary, Dr. S. K. Taheruodin Ahmed, and Mr. Ankit Negi

Second row, (L to R): Mr. Ajay Sharma, Mr. Khem Bahadur, Dr. Ashoke Maity, Mr. Amit Lochab, and Mr. Harpreet Singh

Publications

2023 (Till July 31, 2023)

1. A. Nath, S. Chawla, **A. K. De**, P. Deria, S. Mandal. Inter-Network Charge-Transfer Excited State Formation Within a Two-fold Catenated Metal–Organic Framework. *Chem. Eur. J.*, **2023**, 29(2), 202202978.
2. A. Gogia, H. Bhambri, **S. K. Mandal**. Exploiting a Multi-Responsive Oxadiazole Moiety in One Three-Dimensional Metal–Organic Framework for Remedies to Three Environmental Issues. *ACS Appl. Mater. Interfaces*, **2023**, 15(6), 8241-8252.
3. A. Chanda, **S. K. Mandal**. Selective and ultrafast sensing of 246-trinitrophenol - A nitro-explosive and mutagenic pollutant - In aqueous media by highly stable and recyclable metal-organic probes: Design principles and mechanistic studies. *Dyes Pigments*, **2023**, 210(1), 111025.
4. A. Devi, S. Yadav, **A. K. De**. Complementing two-photon fluorescence detection with backscatter detection to decipher multiparticle dynamics inside a nonlinear laser trap. *Sci. Rep.*, **2023**, 13(1), 739.
5. B. Patel, R. Ranjan, N. R. Chauhan, S. Mukhopadhyay, **A. R. Choudhury**, K. M. Vyas. N-coordinated Ru(II) catalyzed solvent free N-alkylation of primary amines with alcohols through borrowing hydrogen strategy. *New J. Chem.*, **2023**, 47(17), 8305-8317.
6. **B. Devi**, S. M. Arumugam, S. Kumar, **S. Mahala**, S. Elumalai. Thermodynamic Insights into MgBr₂-Mediated Glucose Interconversion to Fructose Undertaking Multiple Reaction Pathways by Applying the Macro- and Micro-Kinetic Principles. *ACS Sustainable Chem. Eng.*, **2023**, 11(8), 3284-3296.
7. C. S. Srinivas, G. S. Singaraju, V. Kaur, S. Das, S. K. Ghosh, A. Sagar, A. Kumar, T. Bhatia, **S. Rakshit**. Transient interactions drive the lateral clustering of cadherin-23 on membrane. *Commun. Biol.*, **2023**, 6(1), 293.
8. C. K. Mahesha, S. A. Borade, D. Tank, K. Bajaj, H. Bhambri, **S. K. Mandal**, R. Sakhuja. Tandem Transformation of Indazolones to Quinazolinones through Pd-Catalyzed Carbene Insertion into an N-N Bond. *J. Org. Chem.*, **2023**, 88(3), 1457-1468.
9. D. Gupta, A. K. Gaur, S. K. Thakur, **S. Singh**, **S. Venkataramani**. Photoswitchable Cu(II) and Cu(I) Complexes of Phenylazo-35-dimethylpyrazole Incorporated Ligands. *Chem. Photo. Chem.*, **2023**, 7, e202200338.
10. A. Mahadevan, P. Kumar, S. Singh, and **S. Venkataramani**. Photochemistry of 2-Iodobenzothiazole and Iodine-Triggered 2-Isocyanophenylthiyl Radical Cyclization in Argon Matrices. *J. Org. Chem.*, **2023**.
11. D. Gupta, A. K. Gaur, H. Kumar, S. Singh, **S. Venkataramani**. Light Switchable Metal Complexes: Introducing Photoresponsive Behaviour Through Azoheteroarenes. *Chem. Photo. Chem.*, **2023**, e202300068.
12. A. Srivastava, S. Grewal, S. Singh, Rajani, **S. Venkataramani**. Photoswitchable Rhodamine-Based Multi-analyte Sensors for Metal Ions Detection. *Chem. Photo. Chem.*, **2023**, e202300029.
13. A. K. Gaur, D. Gupta, A. Mahadevan, P. Kumar, H. Kumar, D. N. Nampoothiry, N. Kaur, S. K. Thakur, **S. Singh**, T. Slanina, and **S. Venkataramani**. Bistable Aryl Azopyrazolium Ionic Photoswitches in Water. *J. Am. Chem. Soc.*, **2023**, 145, 19, 10584–10594.
14. D. P. Singh, A. Shah, I. Bala, V. Marichandran, **S. K. Pal**, A. K. Srivastava, S. Kumar. Organic electronic applications and charge transport mechanism in novel discotic liquid crystals. *Liq. Cryst.*, **2023**, 45140.
15. E. Shandilya, **S. Maiti**. Self-Regulatory Micro- and Macroscale Patterning of ATP-Mediated Nanobioconjugate. *ACS Nano*, **2023**, 17(5), 5108-5120.
16. G. Singh, S. Sharma, R. Pandey, Rekhaa, **R. V. Anand**. Construction of heterocycle-fused tetrahydrocarbazoles through a formal [3 + 3]-annulation of 2-indolylmethanols with para-quinone methides. *Org. Biomol. Chem.*, **2023**, 21(12), 2493-2498.
17. H. Moorthy, M. Yadav, N. Tamang, S. K. Mavileti, L. Singla, **A. R. Choudhury**, D. Sahal, N. R. Golakoti. Antiplasmodial and Antimalarial Activity of 35-Diarylidene-tetrahydro-2H-pyran-4(3H)-ones via Inhibition of Plasmodium falciparum Pyridoxal Synthase. *Chem. Med. Chem.*, **2023**, 18(1), e202200411.
18. J. Singh, J. Lather, **J. George**. Solvent Dependence on Cooperative Vibrational Strong Coupling and Cavity Catalysis. *Chem. Phys. Chem.*, **2023**, 24(11), e202300016.
19. **J. George**, J. Singh. Polaritonic Chemistry: Band-Selective Control of Chemical Reactions by Vibrational Strong Coupling. *ACS Catal.*, **2023**, 13(4), 2631-2636.

Publications

20. K. Saini, S. Kumar, R. Kaur, **S. A. Babu**, S. Saravanamurugan. Accelerated H₂ activation over Pt/M-ZrO₂ for the reductive amination of levulinic acid esters under benign conditions. *Catal. Sci. Technol.*, **2023**, 13(6), 1666-1676.
21. K. Rani, **S. Sengupta**. Correction: Multi-stimuli programmable FRET based RGB absorbing antennae towards ratiometric temperature pH and multiple metal ion sensing. *Chem. Sci.*, **2023**, 14(12), 3386-3836.
22. L. Singla, A. Kumar, C. M. Robertson, P. Munshi, **A. R. Choudhury**. Investigation of C-F...F-C Interactions Using Experimental and Theoretical Charge Density Analyses. *Cryst. Growth Des.*, **2023**, 23(2), 853-861.
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