Department of

CHEMICAL SCIENCES

2020

Indian Institute of Science Education and Research Mohali

Message from the Director

Each of the Departments at IISER- Mohali periodically brings out a brochure on the profiles of its faculty members, and I am delighted that the Department of Chemical Sciences has prepared this updated version in 2020. With twenty-one Faculty and two DST INSPIRE Faculty members, the Department is flourishing on all fronts since its inception in 2012. Teaching courses for the BSMS, Int-PhD and PhD students cover the various fundamental and advanced concepts in chemistry, comprising inorganic, organic, physical, materials and theoretical chemistry. The Faculty is also actively involved in research activities across the different disciplines, which is evident from the quality and numbers of research papers published in reputed Journals and patents filed. Several of the faculty and students are recipients of prestigious awards that are listed in these pages. I firmly believe that the Department will continue to grow in strength and obtain further accolades in future, and I wish the Faculty, staff members and students all success in their endeavours.

J. Gowrishankar
Director

Message from the Head

It's pleasure to present the activities of the Department. Commencement of chemistry classes at IISER Mohali on Aug 16, 2007 is a historical milestone for the Department. The first ever class at IISER Mohali was the chemistry class delivered by Prof. Ramesh Kapoor, a former faculty of the Department. The Department Chemical Sciences was established in June 2012 by the Board of Governors with the vision of the founder Director Prof. N. Sathyamurthy and we are grateful to the BoG and the founder Director. Prof. K. S. Viswanathan served as the first Head of the Department. All the BS-MS students who join IISER Mohali, undergo training in all branches of science – (chemistry, biology, mathematics and physics) and humanities in their first two years, At the commencement of their third year, students opt for a major in one of the four branches of science. These students are taught various fundamental and advanced level chemistry courses. In their final year, these students also carry out a one-year Master's thesis work. It is a matter of pride for us that many of these students have actually been able to obtain publications based on their Master's research. In addition, the Department also offers PhD and Integrated-PhD programmes. Our faculty pursue quality research in various research areas of chemical sciences. The department also accommodate a good number of summer research students every year, from other institutes and those recommended by the Indian Academy of Sciences (IAS). The students of our Department are also very vibrant and run a very active Chemistry Club 'the Curie Club'. The Department also invites eminent scientists, which exposes the faculty and students to new areas of Chemistry. As a department, we have published more than 500 research articles, filed 15 patent applications and organized many conferences including the 1st Edition of CRIKC Chemistry Conference (2019). I am sure that with active participation of all the students and faculty of the Department, we are on the path to attain greater heights.

S. A. Babu
Head, DCS

Table of contents

Sanjay K. Mandal
Professor
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Laboratory for Metal Organic Coordination Networks

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. He spent next sixteen years in the USA including 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 the 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 (a) multi-step organic synthesis, (b) Schlenk-line and glove box techniques, (c) room temperature, hydro-/solvothermal and microwave synthesis of inorganic and metal-organic frameworks, and (d) high temperature solid state calcination of such frameworks. Various spectroscopic methods (UV-vis, FTIR, NMR, Raman, CD and Fluorescence), thermal analysis (TGA and DSC), microscopic techniques (SEM, TEM, AFM, Fluorescence and Confocal), electrochemistry, gas and vapour sorption measurements, X-ray crystallography (PXRD and SCXRD), and magnetic studies are routinely used for establishing physicochemical properties of the new organic, inorganic and organometallic compounds. The experimental work is aided by in-depth computational (DFT and GCMC) studies. This has resulted in the strategic design of coordination architectures 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 decoding and separation, luminescence, gas and liquid adsorption, magnetism, etc. Our research efforts target alternate solutions to some current issues in the fields of (i) mesh-adjustable molecular sieves and adsorbent coolant (green air-conditioning), (ii) selective gas adsorption studies - storage of hydrogen and methane (next generation fuels), (iii) sequestration and conversion of carbon dioxide (lowering greenhouse effect), (iv) chormogenic and/or fluorogenic sensing of cations, anions and neutral small molecules at the ppm or ppb level, (v) chiral catalysis, and (vi) generation and applications of metal oxides and sulfides in luminescence, photocatalysis and quantum dots.

Selected Publications:

(1) "Modulation of hydrophilicity inside the cavity of molecular rectangles self-assembled under ambient conditions", S. Khullar and S. K. Mandal, *Chem. Comm*., **2020**, *56*, 7913.

(2) "Solvent-Induced Diversification of CdS Nanostructures for Photocatalytic Degradation of Methylene Blue", S. Thakur, P. Das, S. K. Mandal *ACS Appl. Nano Mater.*, **2020**, *3*, 5645.

(3) "A Highly Stable Triazole-Functionalized Metal-Organic Framework Integrated with Exposed Metal Sites for Selective CO_2 Capture and Conversion", V. Gupta and S. K. Mandal, *Chem. Eur. J.,* **2020**, *26*, 2658.

(4) "A Primary Amide-Functionalized Heterogeneous Catalyst for the Synthesis of Coumarin-3-carboxylic Acids via a Tandem Reaction", D. Markad, S. Khullar and S. K. Mandal, *Inorg. Chem.,* **2020**, DOI: 10.1021/acs.inorgchem.0c01178.

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

(6) "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", D. Markad and S. K. Mandal, *ACS Catalysis,* **2019**, *9*, 3165.

(7) "Design and Construction of a Chiral Cd(II)-MOF from Achiral Precursors: Synthesis, Crystal Structure and Catalytic Activity toward C-C and C-N Bond Forming Reactions", V. Gupta and S. K. Mandal, *Inorg. Chem.*, **2019**, *58*, 3219.

(8) "Strategic Construction of Highly Stable Metal-Organic Frameworks Combining Both Semi-Rigid Tetrapodal and Rigid Ditopic Linkers: Selective and Ultrafast Sensing of 4-Nitroaniline in Water", G. Chakraborty, P. Das and S. K. Mandal, *ACS Appl. Mater. Interfaces*, **2018**, *49*, 42406.

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

(10) "Manganese Clusters with Relevance to Photosystem II" S. Mukhopadhyay, S. K. Mandal, S. Bhaduri and W. H. Armstrong, invited review, *Chem. Rev.* **2004**, *104*, 3981.

Samrat Mukhopadhyay
Associate Professor
E-mail: mukhopadhyay@iisermohali.ac.in

Biological Chemistry: Intrinsically Disordered Proteins

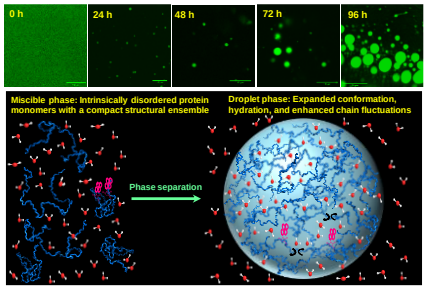
Profile:

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-present/Associate Professor, IISER Mohali
He is also a faculty member at the Centre for Protein Science, Design & Engineering and the Department of Biological Sciences at IISER Mohali

Research Interests:

Proteins are the workhorses of the living systems. Traditionally, protein function was thought to depend on a unique well-defined 3D structure that is encoded by the amino acid sequence. However, current investigations have revealed that a large fraction of the proteome consists of polypeptide segments that lack a well-defined structure under physiological conditions. They belong to a distinct class of proteins termed as intrinsically disordered proteins (IDPs) that challenge the tenets of the traditional structure-function paradigm. The intrinsic disorder in the proteins allows the complex organisms to carry out multiple functions from the same proteins by adopting different conformational states. However, the disorder-to-function relationship is poorly understood. Additionally, dysfunction of many IDPs is associated with a range of deadly diseases such as Alzheimer's disease, Parkinson's disease, Amyotrophic lateral sclerosis (ALS), frontotemporal dementias (FTDs) and cancers.

Our lab utilizes a diverse range of approaches involving biophysics, biochemistry, chemical biology, cell and molecular biology, and advanced single-molecule and ultrafast spectroscopy to gain molecular insights into the conformational ensemble and dynamics, the protein hydration water, liquid-liquid phase separation, aggregation and amyloid formation from various IDPs containing low-complexity and prion-like domains. These studies are beginning to illuminate the unique molecular insights into the pivotal functional and pathological aspects of phase transition of IDPs (see figure).



Upper panel: Time-dependent confocal images of Alexa488-labeled tau K18 showing a transition from a (mixed) dispersed phase (0 h) to droplets with an increase in the number and the size. The fusion events are seen even after 96 h (scale bar 10μ). Lower panel: A depiction of molecular shapeshifting events in phase separation (Ref. 1).

Selected Publications:

1. "Liquid-Liquid Phase Separation is Driven by Large-Scale Conformational Unwinding and Fluctuations of Intrinsically Disordered Protein Molecules" A. Majumdar, P. Dogra, S. Maity & S. Mukhopadhyay* ***J. Phys. Chem. Lett. 2019***, 10, 3929–3936.
2. "Femtosecond Hydration Map of Intrinsically Disordered α-Synuclein" S. Arya, A. Singh, K. Bhasne, P. Dogra, A. Datta,* P. Das,* & S. Mukhopadhyay* ***Biophys. J. 2018,*** 114, 2540–2551.
3. "Synergistic Amyloid Switch Triggered by Early Heterotypic Oligomerization of Intrinsically Disordered α-Synuclein and Tau" K. Bhasne, S. Sebastian, N. Jain, & S. Mukhopadhyay* ***J. Mol. Biol. 2018,*** 430, 2508-2520.
4."Electrostatic lipid-protein interactions sequester the curli amyloid fold on the lipopolysaccharide membrane surface" H.M. Swasthi & S. Mukhopadhyay* ***J. Biol. Chem. 2017***, 292, 19861-19872.
5. "Direct Observation of the Intrinsic Backbone Torsional Mobility of Disordered Proteins" N. Jain, D. Narang, K. Bhasne, V. Dalal, S. Arya, M. Bhattacharya, & S. Mukhopadhyay* ***Biophys. J. 2016***, 111, 768-774.

Sanjay Singh
Associate Professor
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Tel: +91 9878470451

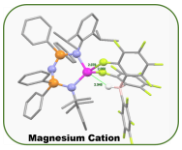
Organometallic & Macrocyclic Chemistry

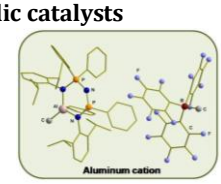
Profile:

PhD – 2003-06/University of Göttingen Göttingen, Germany /Prof. H. W. Roesky
Postdoc–January-November 2006/University of Göttingen, Göttingen, Germany /Prof. H. W. Roesky
Postdoc–December 2006-November 2007/University of Cambridge, Cambridge, U.K. /Prof. D. S. Wright
Professional experience – 2008-16 Assistant Professor, IISER Mohali
2016-present Associate Professor, IISER Mohali

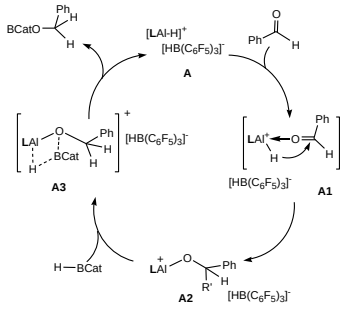
Research Interests:

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

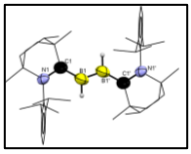


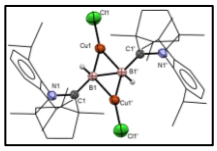


Development of new and efficient environmentally benign main group-based catalysts is the current interest. Synthesis of highly Lewis acidic low coordinated cationic complexes of magnesium, boron and aluminum, supported by bulky ligands with N_2P or N_3P_2 skeleton, is the major emphasis. Applications of these cations in Lewis acid mediated hydroboration (shown below with Al-H cation), hydrosilylation of carbonyls, nitriles and imines have been successfully explored.



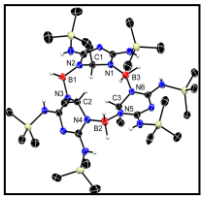
(2) *BICAAC and CAAC carbenes as ligands*: Low valent species (radicals or zero-valent compounds) are of great interests due to their unique electronic structure and high reactivity. Often, these species require kinetic stabilization by the supporting ligand. We exploit strong donor behaviour of CAAC 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.

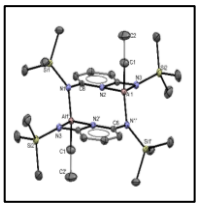




(3) Inorganic macrocycles, pyridinophanes and cryptands

Synthesis of phosph(III)azane based macrocycles and boraamidinate (B-N-B) linked pyridinophanes & cryptands and their Al congeners are major theme of this research area. Use of templates in assembling macrocycles and cryptands (shown below) and host-guest chemistry has opened up new directions.





External Funding:

"*Elucidation of Synthetic Methods, Structural Aspects and Reaction Chemistry of Novel Inorganic Macrocycles and Cryptands*"
Agency: DST EMR; 2017-2019
Amount: INR 52,43,575.

Selected Publications:

(1) "Aluminum Containing Molecular Bowls and Pyridinophanes: Use of Pyridine Modules to Access Different Molecular Topologies" D. Bawari, C. Negi, V. K. Porwal, S. Ravi, K. R. Shamasundar, S. Singh* *Dalton Trans.*, **2019**, 48, 7442.

(2) "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.

(3) "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.

(4) "Neutral and Cationic Cyclic (Alkyl)(Amino)Carbene Mercury [CAAC–Hg(II)] Complexes: Scope of Hydroamination of Alkynes with Organomercury Compounds" D Bawari, B. Goswami, Sabari V. R, S. K. Thakur, R. V. V. Tej, A. R. Choudhury, S. Singh* *Dalton Trans.*, **2018**, 47, 6274.

(5) "A Modular Approach to Inorganic Phosphazane Macrocycles" A. J. Plajer, R. Garca-Rodrguez, C. G. M. Benson, P. D. Matthews, A. D. Bond, S. Singh, L. H. Gade, D. S. Wright *Angew. Chem. Int. Ed.* **2017**, 56, 9087.

(6) "Hg(II) and Pd(II) Complexes with a New Selenoether Bridged Biscarbene Ligand: Efficient Mono- and Bis-arylation of Methyl Acrylate with a Pincer Biscarbene Pd(II) Precatalyst" Rishu, B. Prashanth, D. Bawari, U. Mandal, A. Verma, A. R. Choudhury, S. Singh*, *Dalton Trans.* **2017**, 46, 6291.

(7) "Fine Tuning of Lewis Acidity: The Case of Borenium Hydride Complexes Derived from Bis(phosphinimino)amide Boron Precursors" K. Jaiswal, B. Prashanth, S. Singh*, *Chem.-Eur. J.* **2016**, 22, 11035.

(8) "Two Different Pathways in the Reduction of $[(S=)PCl(\mu\text{-}NtBu)]_2$ with Na" D. Bawari, B. Prashanth, S. Ravi, K. R. Shamasundar, S. Singh*, D. S. Wright *Chem.-Eur. J.* **2016**, 22, 12027. *Hot Paper*.

(9) "Concise Access to Iminophosphonamide Stabilized Heteroleptic Germylenes: Chemical Reactivity and Structural Investigation" B. Prashanth, S. Singh*, *Dalton Trans.* **2016**, 45, 6079.

(10) "Reactivity of a Dihydroboron Species: Synthesis of a Hydroborenium Complex and an Expedient Entry into Stable Thioxo- and Selenoxo-boranes" K. Jaiswal, B. Prashanth, S. Ravi, K. R. Shamasundar, S. Singh*, *Dalton Trans.*, **2015**, 44, 15779.

From Left: first row: Manu Adhikari, Sandeep Rawat, Chandrakala Negi and Mamta Bhandari.

second row: Sandeep Kumar Thakur and Sanjay Singh, Vishal Kumar Porwal and Krishna Kumar Manar

Ramesh Ramachandran
Associate Professor
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Chemical Physics and Spectroscopy

Profile:

Ph.D – 1997-2001/IIT Madras, Chennai /Prof. Mangala Sunder Krishnan
Postdoc – 2001-2007/Massachussets Institute of Technology (MIT), USA /Prof. Robert G Griffin
Professional experience –
2007-2008 –Assistant Professor, IIT Roorkee
2008-2016: Assistant Professor, IISER Mohali
2016-Presemt: Associate Professor, IISER Mohali

Research Interests:

(a) Theory and Methodology development in solid-sate NMR spectroscopy

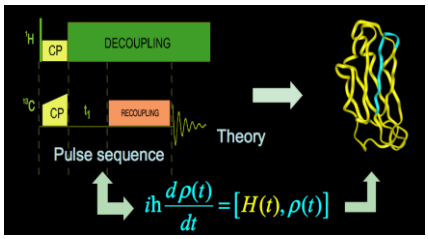
(b) Time dependent Quantum mechanics

(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-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)

Srinivasarao Arulananda Babu
Associate Professor & Head
E-mail: sababu@iisermohali.ac.in
Tel: +91-172-2293165

C-H Activation and Metal-Mediated Organic Synthesis (CAMMOS) Lab

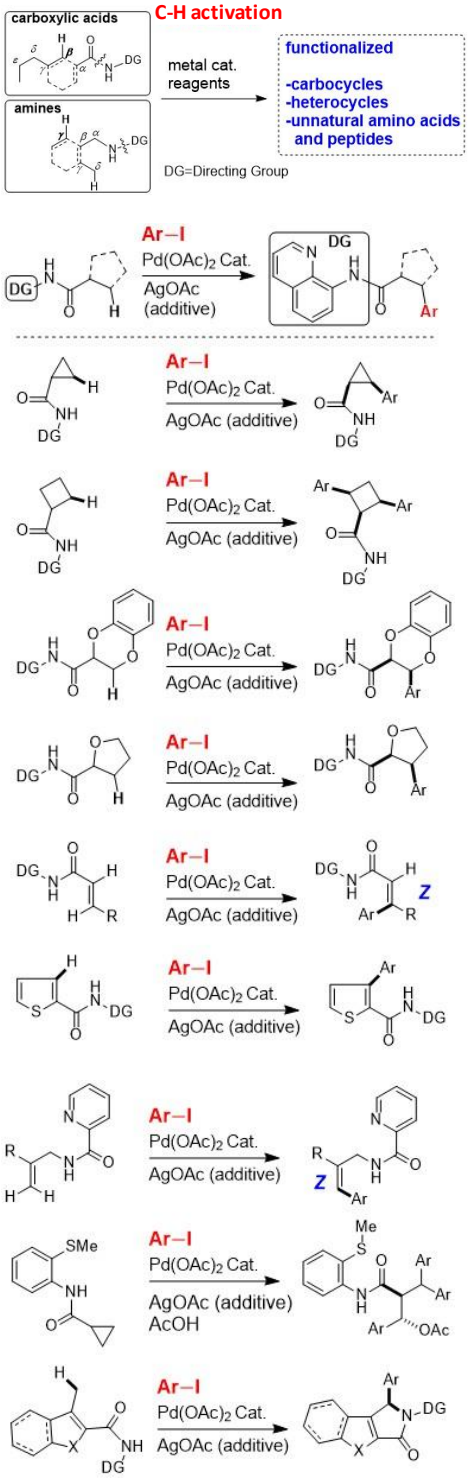
Profile:

Ph.D – 1999-2003/CSMCRI, Bhavnagar, Gujarat, India/Prof. S. Muthusamy.
Postdoc – 2003-2006/Osaka University, Osaka, Japan/Prof. A. Baba.
Professional experience
– Assistant Professor, Mar 2006 - Jan 2009/Osaka University, Osaka, Japan.
–Assistant Professor, Jan 2009 - Mar 2016/IISER, Mohali.
–Associate Professor, Mar 2016 - present.
–Head, DCS, Oct 2017 - present.

Research Interests:

C-H Activation Reactions.
Stereoselective C-C Bond Construction.
Synthesis of Antimalarial Compounds, Unnatural Amino Acids, Macrocycles.
Magnetic catalysis.

Name of the project 1: Strategies toward iminosugars, iminosugar phosphonates, iminosugar C-glycosides (short title). Funding: DST, New Delhi. Fast Track Scheme (Completed, 2013)
Name of the project 2: *Stereoselective C-H Functionalization Route toward Libraries of Bioactive Sugar- and Iminosugar Moieties-Fused Spirooxindoles Scaffolds (short title).*
Funding: CSIR, New Delhi (Completed, 2018)
Name of the project 3: Enantiomerically enriched medium-sized ring-based dibenzoazepine, dibenzoazocine and allocolchicine biaryl alkaloid motifs containing amino acid and amino alcohol backbone *(short title).*
Funding: DST-SERB, New Delhi (2019-, 2018)



Selected Publications:

(1) "Pd-Catalyzed Diastereoselective Intramolecular Amide α-C-H Arylation in Sterically Hindered Monospirooxindole Motifs" Shukla, D., Babu, S. A., *Adv. Synth. Catal.,* **2019**, *361*, 2075.
(2) "Pd(II)-catalyzed sp3/sp2 γ- and δ-C-H functionalization of aryl amines using 5-methylisoxazole-3-carboxamide" Singh, P., Dalal, A., Babu, S. A., *Asian. J. Org. Chem.,* **2019**, *8*, 877.
(3) "Pd(II)-Catalyzed Arylation and Intramolecular Amidation of γ-C(sp3)-H Bonds: En Route To Arylheteroarylmethane and Pyrrolidone-Ring Annulated Furan/Thiophene Scaffolds" Parella, R., Babu, S. A., *J. Org. Chem.,* **2017**, *82*, 7123.
(4) "Pd(II)-Catalyzed, Picolinamide-Assisted, Z-Selective γ-Arylation of Allylamines to Construct Z-Cinnamylamines" Parella, R., Babu, S. A., *J. Org. Chem.,* **2017**, *82*, 6550.
(5) "Diastereoselective Pd(II)-Catalyzed sp3 C-H Arylation Followed by Ring Opening of Cyclopropanecarboxamides: Construction of anti β-Acyloxy Carboxamide Derivatives" Gopalakrishnan, B., Mohan, S., Parella, R., Babu, S. A., *J. Org. Chem.,* **2016**, *81*, 8988.
(6) "Regio- and Stereoselective Pd-Catalyzed Direct Arylation of Unactivated sp³ C(3)-H Bonds of Tetrahydrofuran and 1,4-Benzodioxane Systems" Parella, R., Babu, S. A., *J. Org. Chem.,* **2015**, *80*, 2339.
(7) "Auxiliary-Enabled Pd-Catalyzed Direct Arylation of Methylene C(sp³)-H Bond of Cyclopropanes: Highly Diastereoselective Assembling of Di- and Trisubstituted Cyclopropane-carboxamides" Parella, R., Gopalakrishnan, B., Babu, S. A., *Org Lett.*, **2013**, *15*, 3238.

Patent Applications:
(a) 2811/DEL/2011. (b) 3532/DEL/2012.
(c) 295/DEL/2013. (d) 1102/DEL/2013.
(e) 1240/DEL/2013. (f) 2152/DEL/2013.
(g) 3400/DEL/2013.

Ramasamy Vijaya Anand
Associate Professor
E-mail: rvijayan@iisermohali.ac.in
Tel: +91 9780659432

Synthetic Organic Chemistry

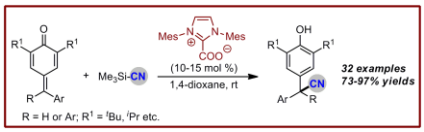
Profile:

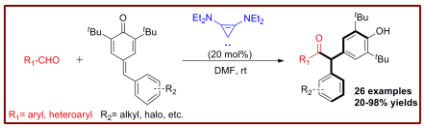
Ph.D – 1997-2003/IIT Kanpur, UP, India /Prof. Vinod K. Singh
Postdoc – 2004-2005/University of Strathclyde, Glasgow, UK/Prof. John A. Murphy
Postdoc – 2006/Texas A&M University, College Station, USA/Prof. Brian T. Connell
Professional experience – 2006-2009/Scientist/Dr. Reddy's Laboratories Ltd/ Hyderabad/India.
Positions held: 2010-1016/Assistant Professor/IISER Mohali
Current Position – Associate Professor (Since March 2016)

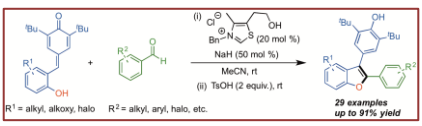
Research Interests:

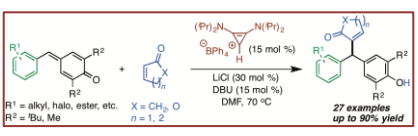
1) Organocatalytic Transformations

Our group is primarily interested in developing organocatalytic transformations using N-heterocyclic carbene (NHC) or bis(amino)-cyclopropenylidene carbene (BAC) based catalysts.



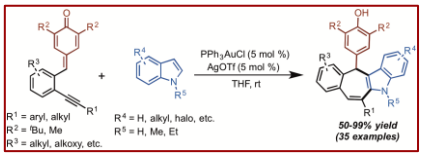


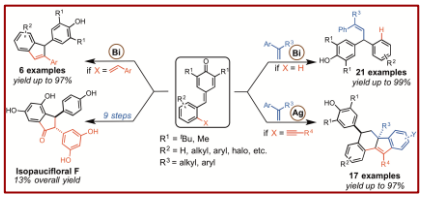


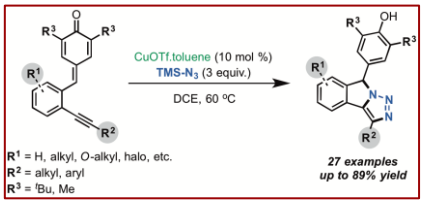


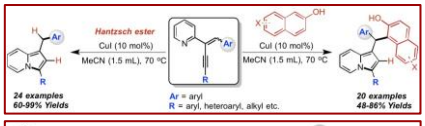
2) Metal-catalyzed Domino Cyclization reactions

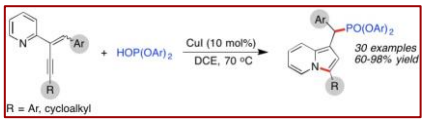
we have developed several methods for the synthesis of unsymmetrical diarylindolylmethanes through metal catalyzed cyclization of 2-alkynylphenyl substituted *p*-QMs with various nucleophiles.











Group Members

Group photo was taken in July 2019 [8 Graduate students and 8 Summer project students]

Selected Publications:

(1) "Base Mediated One-pot Synthesis of Oxygen Based Heterocycles from 2-Hydroxyphenyl-substituted *p*-Quinone Methides" *J. Org. Chem*. **2019**, *84*, 15978.

(2) "A Cascade Synthesis of Hetero-arylated Triarylmethanes Through a Double 5-*endo*-dig Cyclization Sequence" *Chem. Asian. J*. **2019**, *14*, 4688.

(3) "1,6-Hydroolefination and Cascade Cyclization of *p*-Quinone Methides with Styrenes: Total Synthesis of (+/-)-Isopaucifloral" *J. Org. Chem*. **2018**, *83*, 10107.

(4) "A One-pot Approach to 2,3-Diarylbenzo[*b*]furans Through N-Heterocyclic Carbene Catalyzed 1,6-Conjugate Addition Followed by Acid Mediated Dehydrative Cyclization" *J. Org. Chem.* **2018**, *83*, 10546.

(5) "Exploring Gold Catalysis in 1,6-Conjugate Addition-Domino Electrophilic Cyclization Cascade: Synthesis of Cyclohepta[*b*]indoles" *J. Org. Chem*. **2018**, *83*, 8615

(6) "Bis(amino)cyclopropenylidene catalyzed Rauhut-Currier reaction between α,β-unsaturated carbonyl compounds and *para*-quinone methides" *J. Org. Chem.* **2018**, *83*, 4213.

(7) "N-Heterocyclic carbene catalyzed 1,6-conjugate addition of Me_3Si-CN to *para*-quinone methides and fuchsones: Access to α-arylated nitriles" *Org. Lett.* **2017**, *19*, 1982.

(8) "Bis-(amino)cyclopropenylidene-catalyzed 1,6-conjugate addition of aromatic aldehydes to *p*-quinone methides: Expedient access to α,α'-diarylated ketones" *Org. Lett*. **2015**, 17, 3952.

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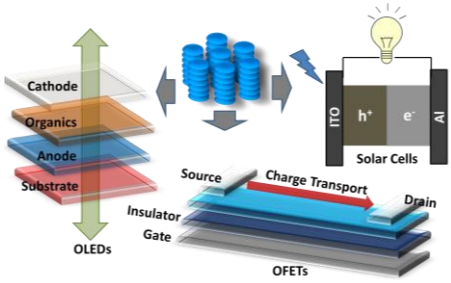
Supramolecular Chemistry

Profile:

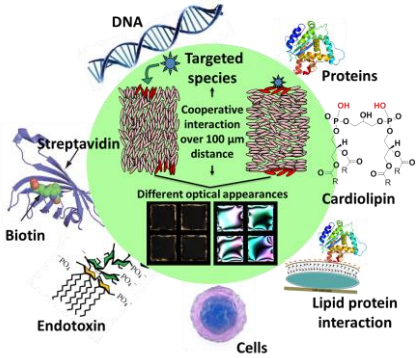
PhD – 2003-08/Raman Research Institute, Bangalore, India
Postdoc – 2008-10/University of Wisconsin, Madison, USA
Professional experience– 2010-2016/Assistant Prof. /IISER Mohali.
2016-present/Associate Prof. /IISER Mohali.

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) "High Hole Mobility and Efficient Ambipolar Charge Transport in Heterocoronene-Based Ordered Columnar Discotics" J. De, I. Bala, S. P. Gupta, U. K. Pandey, **S. K. Pal*** *J. Am. Chem. Soc.* **2019**, 141, 18799.
(2) "Natural sunlight driven oxidative homocoupling of amines by truxene based CMP" V. R. Battula, H. Singh, S. Kumar, I. Bala, **S. K. Pal***, K. Kailasam *ACS Catal.* **2018**, 8, 6751.
(3) "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.
(4) "Proton-Triggered Fluorescence Switching in Self-Exfoliated Ionic Covalent Organic Nanosheets for Applications in Selective Detection of Anions" H. Singh, M. Devi, N. Jena, M. M. Iqbal, Y. Nailwal, A. D. Sarkar, **S. K. Pal*** *ACS Appl. Mater. Interfaces*, **2020**, DOI: 10.1021/acsami.9b20743.
(5) "Room-Temperature Columnar LCs as Efficient Pure Deep-Blue Emitters in Organic Light-Emitting Diodes with an EQE of 4.0%" J. De, W. Y. Yang, I. Bala, S. P. Gupta, R. A. K. Yadav, D. K. Dubey, A. Chowdhury, J. H. Jou, **S. K. Pal*** *ACS Appl. Mater. Interfaces*, **2019**, 11, 8291.
(6) "Design of Aqueous-LC Interfaces To Monitor Protein Aggregation at Nanomolar Concentrations" I. Pani, H. M. Swasthi, S. Mukhopadhyay, **S. K Pal*** *J. Phys. Chem. C*, **2019**, 123, 1305.
(7) "A new strategy towards the synthesis of a RT discotic nematic LC employing triphenylene and pentaalkynylbenzene units" M. Gupta, S. P. Gupta, M. V. Rasna, D. Adhikari, S. Dhara, **S. K. Pal*** *Chem. Commun.* **2017**, 53, 3014.
(8) "LC based Detection of Pb(II) ions using Spinach RNA as Recognition Probe" I. Verma, M. Devi, D. Sharma, R. Nandi, **S. K. Pal*** *Langmuir*, **2019**, 35, 7816.

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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 –

i) 2008-2010/Biocon-BMS Research Center (BBRC), Bangalore.
ii) 2010-11/Jubilant Biosys Ltd, Bangalore.
iii) 2011-2017/Assistant Professor, IISER Mohali
iv) 2017-till/Associate Professor, IISER Mohali

Research Interests:

Our research primarily centres on the following areas:

- Development of stereoselective reactions with particular emphasis on
(i) Brønsted and Lewis acid catalysis
(ii) Asymmetric organocatalysis involving small molecule amines and phosphines

- Development of sustainable and atom economic reactions.

Application of aforementioned strategies in the total synthesis of architecturally complex bioactive natural products and pharmaceutically important compounds.

- Emphasis 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

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

Our webpages

http://14.139.227.202/faculty/sastry/

http://www.iisermohali.ac.in/faculty/dcs/ramsastry

Back row: Nitul, Ramasastry, Prashant, Atanu, Jay Prakash, Kaushalendra
Front row: Lona, Ketankumar, Uttam, Bara Singh, Sonu, Dipto

Selected Publications:

(1) 'Palladium-Catalyzed Intramolecular Trost-Oppolzer-Type Alder-Ene Reaction of Dienyl Acetates to Cyclopentadienes' Bankar, S. K.; Singh, B.; Tung, P.; Ramasastry, S. S. V. *Angew. Chem. Int. Ed.* **2018**, *57*, 1678.
(2) 'One-Pot Trimetallic Relay Catalysis: A Unified Approach for the Synthesis of *β*-Carbolines and Other [*c*]-Fused Pyridines' Dhiman, S.; Mishra, U. K.; Ramasastry, S. S. V. *Angew. Chem. Int. Ed.* **2016**, *55*, 7737.
(3) 'Morita-Baylis-Hillman Reaction of *β,β*-Disubstituted Enones: An Enantioselective Organocatalytic Approach for the Synthesis of Cyclopenta[*b*]annulated Arenes and Heteroarenes' Satpathi, B.; Ramasastry, S. S. V. *Angew. Chem. Int. Ed.* **2016**, *55*, 1777.
(4) 'Organophosphine Catalyzed Intramolecular Hydroacylation of Activated Alkynes' Mondal, A.; Hazra, R.; Grover, J.; Raghu, M.; Ramasastry, S. S. V. *ACS Catal.* **2018**, *8*, 2748.
(5) 'Metal- and Hydride-Free Pentannulative Reductive Aldol Reaction' Satpathi, B.; Dutta, L.; Ramasastry, S. S. V. *Org. Lett.* **2019**, *21*, 170.
(6) 'Synthesis of Cyclopropanoids via Substrate-Based Cyclization Pathways' Mishra, U. K.; Patel, K.; Ramasastry, S. S. V. *Org. Lett.* **2019**, *21*, 175.
(7) 'Substituent-Guided Palladium-Ene Reaction for the Synthesis of Carbazoles and Cyclopenta[*b*]indoles' Yadav, S.; Hazra, R.; Singh, A.; Ramasastry, S. S. V. *Org. Lett.* **2019**, *21*, 2983.
[8] 'Organocatalytic β-Azidation of Enones Initiated by an Electron-Donor-Acceptor Complex' Shirke, R. P.; Ramasastry, S. S. V. *Org. Lett.* **2017**, *19*, 5482.

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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.

Research Interests:

Synthesis, Characterization and Solid State Chemistry of Small Organic Molecules and Metal-organic Frameworks:

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.

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 nitrogen based linkers are being used for the generation of MOFs in our laboratory.

Funding : IISER Mohali (2009-ongoing)
Contributors: Dr. Gurpreet Kaur, Dr. Prasanta Bhowmik, Dr. Hare Ram Yadav, Dr. Dhiraj Das.

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.

Funding: DST and IISER Mohali (2009-ongoing)
Contributors: Mr. Maheswararao Karanam, Ms. Indu Verma, Mr. Mayank Joshi.

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

Weak interactions in the solid state are best studied by analysing the electron densities associated with the said interaction through experimental charge density determination and theoretical calculation of the same. Through this analysis, we can quantify the electron densities in the intermolecular regions in the solid state and can comment on the nature of such interactions.

Funding : IISER Mohali (2009-ongoing).
Contributor: Dr. Gurpreet Kaur, Dr. Hare Ram Yadav and Ms. Labhini Singla.

Current Lab Members
From Left: Mayank Joshi, Manish Kumar Yadav, Angshuman Roy Choudhury, Dhiraj Das and Labhini Singla

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.

Funding: IISER Mohali (2011-till date).
Contributors: Dr. Gurpreet Kaur, Mr. Maheswararao Karanam.

Selected Publications:

(1) "Water-assisted ground state intra-molecular proton transfer in 2,5-dihydroxy-substituted azobenzenes: experimental and computational studies", Das, D.; Choudhury, A. R. *CrystEngComm.* **2019**, *21*, 2373-2380.
(2) "Salts of Amoxapine with Improved Solubility for Enhanced Pharmaceutical Applicability", Joshi, M.; Choudhury, A. R. *ACS Omega*. **2018**, *3*, 2406-2416.
(3) "Structural and computational understanding of weak interactions in "bridge-flipped" isomeric tetrafluoro-bis-benzylideneanilines". Dhingra, S.; Barman, D. J.; Yadav, H. R.; Eyyathiyil, J.; Bhowmik, P.; Kaur, P.; Adhikari, D.; Choudhury, A. R. *CrystEngComm.* **2018**, *20*, 716-727.
(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:

Electron-correlation methods for open-shell molecules:

We have recently developed a internally contracted multi-reference (ICMR) method and demonstrated its efficiency and applicability for moderate-size inorganic open-shell molecules. Our current focus is to develop (a) an ICMR method for simultaneous treatment of several excited states (b) analytic gradients and non-adiabatic couplings for ICMR methods (c) novel ICMR coupled-cluster methods.

Photochemistry of α-β enones.

Our research is aimed at understanding some aspects of photochemistry of α–β enones. Fermto-second experiments have revealed surprisingly different ultrafast electronic quenching for different methyl substituted Acroleins. We have made a comparative study of Acrolein and Crotonaldehyde excited state dynamics following photo-excitation to π-π* S2 state. We are using a semi-classical excited state dynamics method to understand the differences in non-adiabatic population transfer in these molecules. Contributors: Satyam Ravi (Ph.D. student).

Electron impact ionization of small molecules.

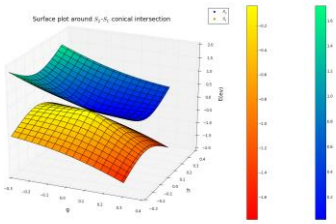
We have carried out a comparative study of charge symmetric dissociation of dications of N_2 and CO molecules, by computing potential energy curves for several states contributing to the experimentally observed KER pattern. Contributor: K. R. Shamasundar, Dr.Bhas Bapat and Dr.Amredra Pandey from PRL, Ahmedabad.

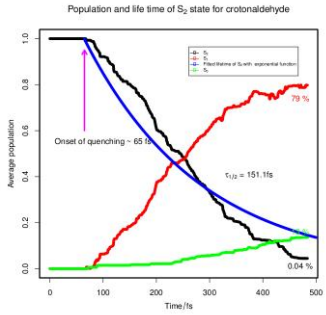
Molecular Properties using Fock-space coupled-cluster methods.

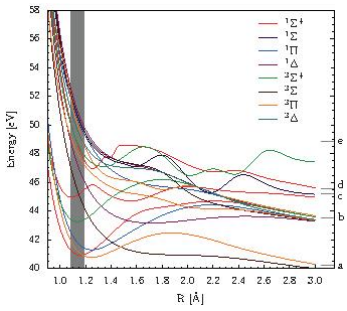
We are implementing a recently developed method for the analytic computation of molecular properties using a new formulation of FSCC theory. We expect this to be a cheap and useful alternative method to investigate electronic states near the Franck-Condon region. We have developed a new symbolic manipulation toolbox for automatic derivation of equations of quantum chemistry. Contributors: Dr. Jitendra Gupta.

Computational Study of molecules containing Boron.

Recently, we have applied ab initio methods to explain the properties of a rare example containing Boron-Sulphur double bond. Computational studies of unknown cyclic four-membered Boron based systems have also been carried out. Contributors:. Pratip Chakraborty (MS Student) and Satyam Ravi, in collaboration with the experimental group of Dr.Sanjay Singh.



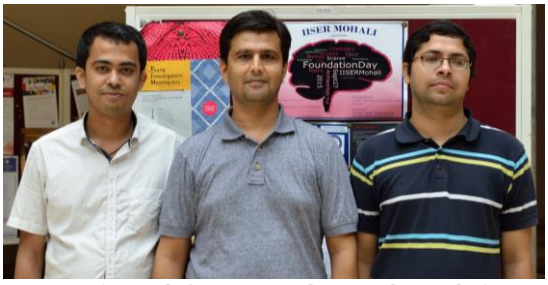




Selected Publications:

(1) Jaiswal, K; Billa, P; Satyam Ravi; Shamasundar, K. R; Sanjay Singh., *Dalt. Trans.* **2015**, *44*, 15779.

(2) Pandey, A. K; Bapat, B; Shamasundar, K. R., *J. Chem. Phys.* **2014,** *140*, 034319.



(From left: Satyam, Sham and Jitendra)

Sugumar Venkataramani
Assistant Professor
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Tel: +91 9915323141

Physical Organic Chemistry

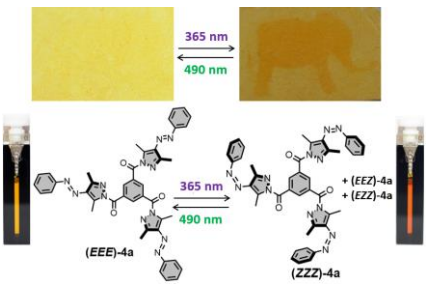
Profile:

Ph.D – 2003-07/Ruhr University Bochum, Germany/Prof. Wolfram Sander
Postdoc – 2008-09/CA University Kiel/AvHumboldt fellowship/Prof. Rainer Herges
Professional experience – 2010-13/Orchid Pharma, Chennai/Research Scientist

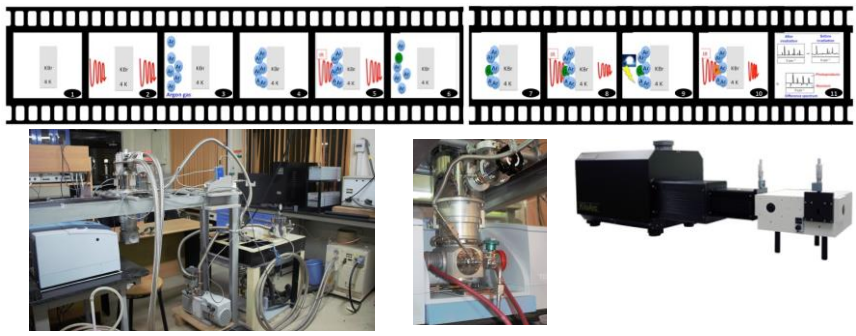
Research Interests:

Photoswitchable Functional Molecules: (Funding: Start up & SERB, 2015 – 2019, EMR/2014/0000780**)**
Utilizing the concepts of photoswitching behaviour, simple and molecules containing multiple azoarenes are designed and synthesized. Various studies ranging between fundamental aspects like substituent effects to applications such as encapsulation and release of guest molecules are being investigated. Multiple spectroscopic techniques and computations are the major tools. The long-term goals are drug delivery and time -bound encapsulation, catalysis etc.

Chem. Eur. J., **2019**, 10.1002/chem.201902150



ChemPhotoChem, **2018**, 2, 806-810



Matrix isolation infrared spectroscopic and computational studies of reactive intermediates: (Funding : Start up**)**
One of our major interests is to understand the structure, stability and reactivity of radicals and highly reactive species. 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 presursors with photo-labile 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) "Evaluation of Substituent Effect in Z-Isomer Stability of Arylazo-1H-3,5-dimethylpyrazoles – Interplay of Steric, Electronic Effects and Hydrogen Bonding" Sudha Devi, Mayank Saraswat, Surbhi Grewal, Sugumar Venkataramani* *J. Org. Chem.*, **2018**, 83, 8, 4307-4322.
(2) "Does a nitrogen lone pair lead to two centered-three electron (2c-3e) interactions in pyridyl radical isomers?" Chitranjan Sah, Lilit Jacob, Mayank Saraswat, Sugumar Venkataramani, *J. Phys. Chem. A,* **2017**, *121*, 3781-3791.
(3) "Dehydro-oxazole, thiazole and imidazole radicals: Insights into the electronic structure, stability and reactivity aspects" Anamika Mukhopadhyay, Lilit Jacob, Sugumar Venkataramani, *Phys. Chem. Chem. Phys* , **2017**, *19*, 394-407.

Group Members:
(From left): Himanshu Kumar, Ankit Somani (completed MS), Ankit Gaur, Chitranjan Sah, Anjali Mahadevan, Dr. Sudha Devi (graduated), Virender Singh (completed MS), Surbhi Grewal, Pravesh Kumar, Anjali Srivastava, Debapriya Gupta, Mayank Saraswat
(Insert: Amandeep Singh, Sonam Suwasia, Lincoln, Anees Rahman P)

Balanarayan P
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Computational and Theoretical 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. **Chemical Reactions in high frequency strong oscillating fields**

Atoms and molecules in strong high frequency oscillating fields exhibit interesting stabilization characteristics. The stable states formed in the presence of high intensity lasers of electric field strength of the order of 10^{11} to 10^{14} W/cm^2 have a strongly polarized and highly reactive nature. This project specifically deals with the possibility of realizing new chemical reactions in the stabilized regime.

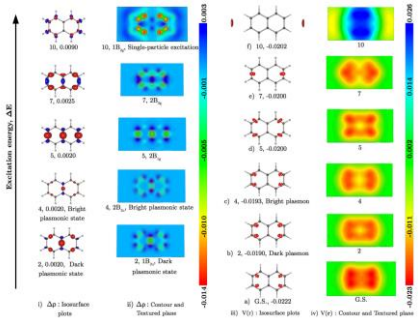

Figure: Molecular Plasmons

Molecular plasmons: Characteristics of

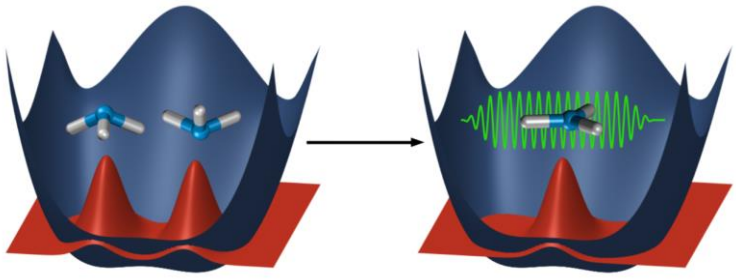

Figure: Ammonia in strong laser fields

Ammonia molecule in a high intensity high frequency laser

Our Ph.D. student Naveen Kumar is currently looking at a problem, which involves the stabilization of ammonia molecule on top of the double well barrier using a high intensity and high frequency laser. It has been found that the planar geometry of ammonia is more stable than the pyramidal one at particular frequencies and intensities of the CW laser with the laser polarization along the C_3 axis of ammonia. In our project we are currently probing how the planar geometry is realized in a CW laser and what are its experimental signatures.

From the left/front: Harwinder, Kirti, Mishu, Arghadeep, Taseng, Alkit, Sourav, Nitin, Prateek, Naveen, Gokul, and Prashant

Methodology development in quantum dynamics: Programs for electronic time propagation

Properties of atoms and molecules and general computational chemistry: The analysis of structure and properties atoms and molecules has been followed by Nitin Kumar Singh and Mishu Paul.

Selected Publications:

(1) "Linear Stark effect for a sulfur atom in strong high frequency laser fields" P. Balanarayan, N. Moiseyev, *Phys. Rev. Lett.* **2013**, 110, 25301.
(2) "Strong chemical bond of stable He_2 in strong linearly polarized laser fields" P.Balanarayan and N. Moiseyev, *Phys. Rev A* **2012**, 85, 032516.
(3) "Can ring strain be realized in momentum space?" P. Balanarayan and S. R. Gadre *J. Amer. Chem. Soc.*, **2006**, 128, 10702.

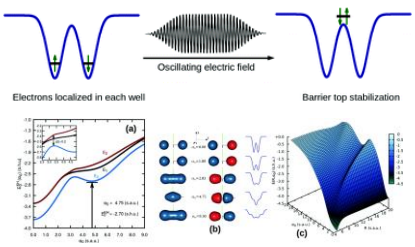

Figure: A Balancing act of two electrons in an oscillating field

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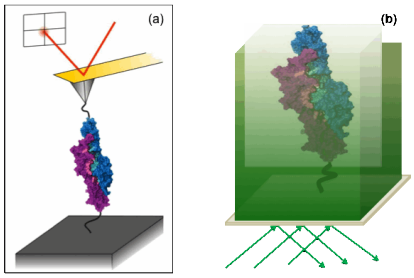
Nanomechanics of Biomolecules

Profile:

Ph.D – 2003-09/Indian Institute of Science, Bangalore, India /Prof. S. Vasudevan.
Postdoc – 2009-13/Iowa State University, Ames, USA /Prof. S. Sivasankar

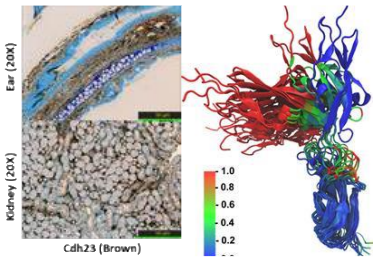
Research Interests:

Deciphering the 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 stereocillia. 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 stereocillia. 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. We are particularly interested in (a) understanding the binding kinetics of the proteins forming tip-links against tensile force and their reproducibility, (b) measuring the molecular elasticity of these proteins etc. We will further extend these studies with mutant proteins leading to deafness or Usher Syndrome.

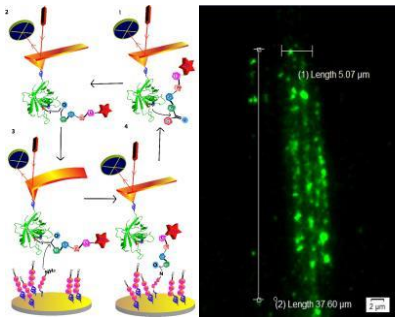
Funding : DBT-Wellcome Trust Intermediate Fellowship (Awarded, 2015)



Cadherins in Cancer

Cadherin-23, a cell adhesion protein, belongs to the family of non-classical cadherins. CDH23 through its outer most extra-cellular domains interacts homophilically and heterophilically with its binding partners. Recent reports have shown that the localization of CDH23 at the cell-cell junctions of cancer cells might play a role in early metastasis. TCGA analysis of CDH23 expression at mRNA level suggested that many cancers showed down-regulation of CDH23 expression at stage 4 compared to other stages, in metastasis (M1) stage and the patients having higher expression of CDH23 has better survival rate. We hypothesized that CDH23 is mediating strong cell-cell adhesion leading to increased tumour size in initial stages of cancer, however, it's strong adhesiveness is inhibiting metastasis leading to better survival of patients. We are interested in a) finding the variation in the expression of different isoforms of CDH23 at m-RNA and protein level in different cancer cells, b) measuring the strength of interactions mediated by CDH23 at single molecule and single cell level, and, c) elucidating the role of CDH23 in cell migration. We will continue to study the biological function of CDH23 at different perspectives.

Trapping Reaction-Intermediate at the single molecule level



We have developed a technique to trap enzymatic reaction intermediate at the single molecule level with an AFM cantilever. This trapping not only helps us understand the kinetics of a reaction at the molecular level but also allows us to print or write anything on a substrate molecule by molecule with sub-nanometer precision. Using AFM cantilever as a 'Pen' here, we are able to create patterns with biomacromolecules and small molecules.

Selected Publications:

(1) "Strong Aggregation-propensity of Cadherin-23 inhibit cell migration." Malay K. Sannigrahi, Sai Srinivas, Nilesh Deokate and Sabyasachi Rakshit. *Molecular Oncology (2019)*.
(2) "Force-activated catalytic pathway accelerates bacterial-adhesion against flow." Jagadish P. Hazra, Nisha Arora, Amin Sagar, Shwetha Srinivasan, Abhishek Chaudhuri, and Sabyasachi Rakshit. *Biochem. J. (2018).*

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Experiment (Ultrafast spectroscopy and Optical trapping)
Theory (Numerical simulation of excited-state dynamics and optical force)

Profile

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

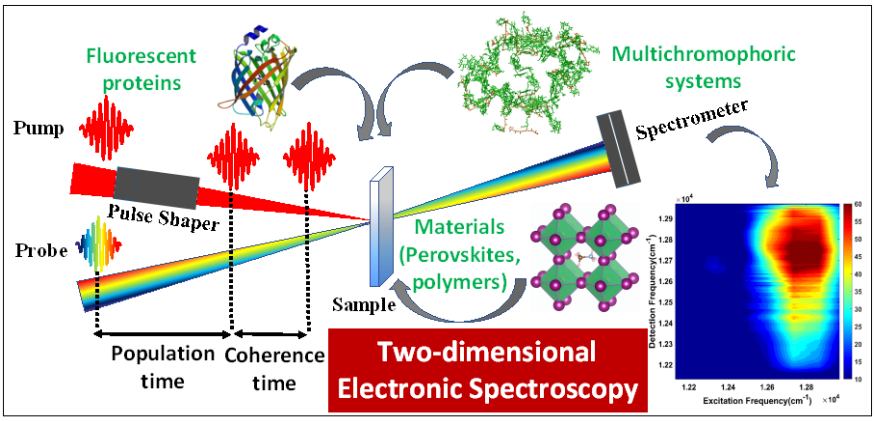
Postdoc– 2010-14/Lawrence Berkeley National Laboratory/University of California Berkeley/Prof. G. R. Fleming

Research Interests

We love to pursue any research problem that excites us and, being optical spectroscopists, we try to solve the problem by "shedding light on them". In particular, we plan to develop novel time-resolved optical spectroscopic and microscopic tools to explore a wide range of interesting physical, chemical and biological phenomena in condensed phase (for example, primary processes in photosynthesis).

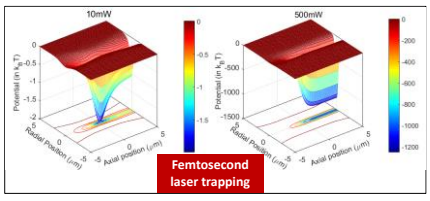
We wish to study (and, hopefully, control!) coherent energy/charge transfer dynamics within natural light harvesters (for example, photosynthetic pigment-protein complexes, fluorescent proteins) as well as within their artificial analogues (for example, molecular aggregates, photovoltaic materials) using femtosecond two-dimensional electronic spectroscopy which are supported by theory of excited-state dynamics.

Using an AOPDF pulse-shaper, we have set up a two-dimensional electronic spectrometer to explore a multitude of interesting problems, as outlined in the schematic below:



We also wish to understand nano-scale optical forces using femtosecond laser tweezers for which we have developed theoretical models to include nonlinear optical effects to estimate force/potential.

We were the first to show how optical trapping potential is dramatically modulated under femtosecond pulsed excitation as shown in the figure below:



We have designed and built a completely table-top versatile optical tweezer set-up with multimodal detection:

A) wide-field detection mode to record both bright-field and dark-field images

B) point detection mode to simultaneously detect both two-photon fluorescence and back-scatter

For more details, please visit our research group website:

https://sites.google.com/site/akdegroupiisermohali/

Funding:

IISER Mohali (Start-up grant)

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

Selected Publications

(1) "Early time solvation dynamics probed by spectrally resolved degenerate pump-probe spectroscopy" Y. Silori, P. Seliya and A. K. De, *ChemPhysChem*, **2019**, 20, 1488.

(2) "Towards CdZnTe solar cells: An evolution to post-treatment annealing atmosphere" S. Chander, A. K. De and M. S. Dhaka, *Solar Energy*, **2018**, 174, 757.

(3) "Theoretical estimation of optimal parameters for maximum fluorescence under pulsed excitation" M. Kayanattil and A. K. De, *ChemPhysChem*, **2018**,19, 2796.

(4) "Probing excited state dynamics of Venus: origin of dual-emission in fluorescent proteins" S. Dhamija, B. Thakur, P. Guptasarma and A. K. De, *Faraday Discussions*, **2018**, 207, 39.

(5) "How to study picosecond solvation dynamics using fluorescent probes with small Stokes shifts" Y. Silori, S. Dey and A. K. De, *Chemical Physics Letters* (Frontiers Article), **2018**, 222, 693.

(6) "Theoretical estimation of nonlinear optical force on dielectric spherical particles of arbitrary size under femtosecond pulsed excitation", A. Devi and A. K. De, *Physical Review A*, **2017**, 96, 023856.

(7) "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.

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:

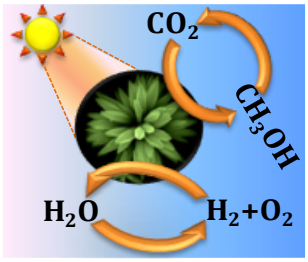
Ph.D – 1999-2006/Indian Institute of Science
Postdoc– 2006-08/National Institute for Materials Science, Tsukuba, Japan
ICYS-Independent researcher-2008-11
Ramanujan Fellow – 2011-14, JNCASR, Bangalore

Research Interests:

Our research works focus on synthesis and characterization of functional nanomaterials and their applications in catalysis, energy harvesting and environmental remediation. We also investigate self-assembly of fullerenes at liquid interfaces and explore their novel physical and chemical properties. Using self assembly for molecular shape shorting is a special goal.

Nanomaterials for energy harvesting and environmental remediation:

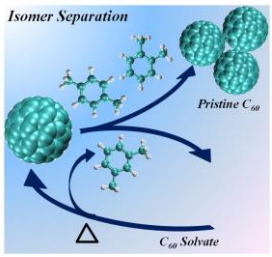
With the daily mean concentrations of atmospheric carbon dioxide having reached 400 parts-per-million for the first time in human history, the need for carbon-neutral alternatives to fossil fuel energy has never been more compelling. Nanomaterials with excellent activity, greater selectivity, and high stability. Their properties can be tuned by tailoring the size, shape, and morphology of the particular nanomaterial. 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 heterogenous catalysts and then evaluate their efficiency toward (a) water splitting and Hydrogen energy harvesting, (b) oxygen reduction or fuel oxidation reaction. (c) We further investigate photochemical or electrochemical conversion of CO_2 to useful chemicals using nanocatalysts. Since many of these catalysts are useful otherwise too, we undertake active collaboration for the development of sustainable protocols for various challenging reactions like C-H activation, C-C coupling, oxidation, hydrogenation, and conversion of pollutants to fine chemicals.



Weak interaction based self-assembly and applications:

Among the carbon allotropes, fullerenes are unique due to their solution processibility and applications in energy harvesting. In the emerging field of carbon based semiconductors, fullerenes are excellent candidates owing to electron accepting nature. We are working towards understanding thechemical interactions involved in such solvates and exploring their effects on the effective electronic properties.

Another purpose of research on this areais to explore their aggregation properties in presence of specific molecules and develop strategies for chemical sensing and molecular shape shorting.



Selected Publications:

(1) "Synthesis of Bi_3TaO_7-Bi_4TaO_8Br composite in ambient air and its high photocatalytic activity upon metal loading", K Chatterjee, M Banoo, S Mondal, L Sahoo, U K Gautam*, Dalton Trans, 2019, 48, 7110.

(2) "Emerging materials in heterogeneous electrocatalysis involving oxygen for energy harvesting", M Rana, S Mondal, L Sahoo, K Chatterjee, P E Karthik, U K Gautam*, ACS Appl. Interface Mater. 2018, 10, 33737.

(3) "C_{60} mediated molecular shape sorting: separation and purification of geometrical isomers" M. Rana, R. Bharathanatha Reddy, B. B. Rath, U. K. Gautam, *Angew. Chem. Int. Ed.* **2014**, 53, 13523.

Group Members:

(From left): Maqsuma, Lipi, Dr. Ujjal, Sandita, Parmeet, Reeya and Sanjit (Inset: Raj)

Debashis Adhikari
Assistant Professor
E-mail: adhikari@iisermohali.ac.in
Tel: +91 9836176798

Synthetic Inorganic, Organometallic, Catalysis

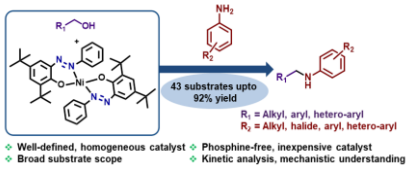
Profile:

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/ Adjunct Lecturer/ Indiana University, Bloomington, IN, USA

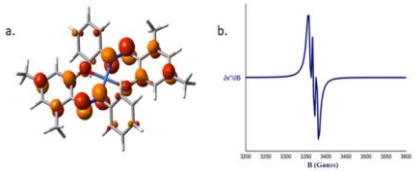
Research Interests:

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

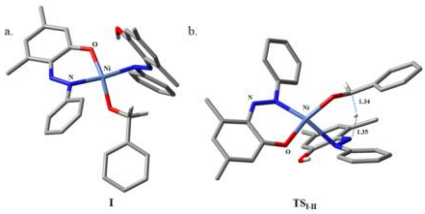
We recently reported a well-defined and bench- stable azo-phenolate ligand coordinated nickel catalyst which can efficiently execute N-alkylation of a variety of anilines by alcohol. We demonstrated that the redox-active azo ligand can store hydrogen generated during alcohol oxidation and redelivered 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.

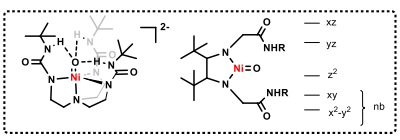


A computational probation (DFT) further provided convincing proof for the HAT step**.** Shown here is an important intermediate along the reaction pathway as well as the transition state for HAT. This example showcases the tandem reactivity of nickel with a redox active ligand.



2. Metal-oxo Chemistry

Another major focus of the group is to synthesize late transition metal-ligand multiple bonded motifs which can trigger C-H bond activation chemistry. These motifs are very challenging to synthesize, and higher oxidation state of the metal is desired to keep the d-electron count low. The bond-activation chemistry of these molecules is intricately connected to their intriguing electronic structure. We will attempt synthesizing late transition metal oxo by suitable ligand design as well as invoking secondary coordination sphere interaction. The structure of a targeted nickel-oxo complex is shown.



Selected Publications:

1) Bains. A. K.; Adhikari. D. *; Mechanistic insight into an azo-radical promoted dehydrogenation of heteroarene towards N-heterocycles. *Cat. Sci. Tech. 2020*, **DOI**: *10.1039/D0CY01008A.*

2) Bains. A. K.; Dey. D.; Yadav. S.; Kundu. A.; **Adhikari. D. *;** Nickel catalysed construction of benzazoles via hydrogen atom transfer reactions. *Cat. Sci. Tech. 2020*, **DOI:** *10.1039/D0CY00748J*.

3) Jana. A.; Das. K.; Kundu. A.; Thorve. P. R.; **Adhikari. D. *;** Maji. B. * A Phosphine-Free Manganese Catalyst Enables Stereoselective Synthesis of (1 + *n*)-Membered Cycloalkanes from Methyl Ketones and 1,*n*-Diols. *ACS Catal.* 2020, 10, 2615.

4) Bains. A. K.; Kundu. A.; Yadav. S.; **Adhikari. D.** * Borrowing Hydrogen-Mediated N-Alkylation Reactions by a Well-Defined Homogeneous Nickel Catalyst. *ACS Catal.* 2019, 9, 9051.

Front row: (from left) Dhananjay, Vikramjeet, Debashis, Amreen
Back row : (from left) Subhankar, Kirti, Vidhyalakshmi, Misbah, Abhishek
Missing : Sudha

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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: 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.

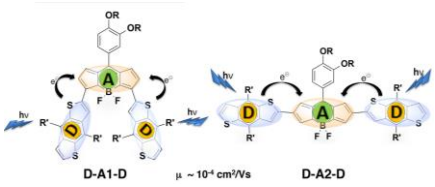

Fig 1. Schematic representation of regioisomeric D-A-D systems with efficient PET and charge carrier mobilities.

2. Multichromophoric Light Harvesting Antenna Systems for Efficient Energy Transfer: Covalently connected multichromophoric systems (based on squaraine, DPP, BODIPY, isoindigo and few other classes of molecules with complementary absorption) with the aim of achieving efficient Förster resonance energy transfer (FRET) will be designed. Design strategies would involve use of scaffolds where chromophores can be positioned with favorable orientations for FRET.

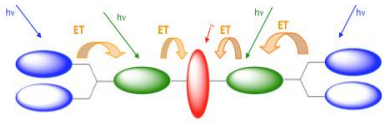

Fig 2. Schematic representation of multichromophoric LH system for FRET.

Eventual aim is to achieve enhanced OPV performances compared to conventional donor-acceptor blends.

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), aggregate induced emission (AIE) and / or thermally activated delayed fluorescence (TADF). Fundamental structure-property relationships of these materials will be deduced through structural and optical characterization. In order to understand the dynamics of various photophysical processes, ultrafast spectroscopic studies would be performed. Eventually, the application of some of the screened materials in fabrication of organic light emitting diodes (OLEDs) will be explored.

4. Computational Investigation of Optical and Redox Properties: Quantum chemical density functional theory (DFT) calculations will be performed on different proposed molecular structures in order to compute their redox and optical properties for efficient molecular design.

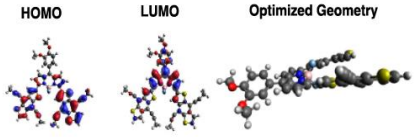

Fig 3. DFT calculated frontier molecular orbitals (FMOs) and optimized geometry of a D-A-D triad.

Selected Publications:

(1)"Regioisomeric BODIPY-Benzodithiophene Dyads and Triads with Tunable Red Emission as Ratiometric Temperature and Viscosity Sensors."
Aswathy P. R., S. Sharma, N. P. Tripathi, S. Sengupta.* *Chem. Eur. J.* **2019** (10.1002/chem.201902952).

(2) "Effect of Structural Isomerism in BODIPY based Donor-acceptor co-polymers on their Photovoltaic Performance."
G. Tarafdar, U. K. Pandey, S. Sengupta*, P. C. Ramamurthy.* *Solar Energy*, **2019**, *186*, 215-224.

(3) "Spectral- and Structural Variations of Biomimetic Light-Harvesting Nanotubes."
A. Löhner, T. Kunsel, M. I. S. Röhr, T. L. C. Jansen, S. Sengupta, F. Würthner, J. Knoester, J. Köhler. *J. Phys. Chem. Lett.* **2019**, *10*, 2715–2724.

(4) "Dual Emissive Bodipy-Benzodithiophene-Bodipy TICT Triad with Remarkable Stokes Shift of 194 nm."
S. Sengupta*, U. K. Pandey. *Org. Biomol. Chem.*, **2018,** *16*, 2033-2038.

(5) "Regioisomeric Donor-Acceptor-Donor triads based on benzodithiophene and BODIPY with distinct optical properties and mobilities."
S. Sengupta*, U. K. Pandey, E. U. Athresh, *RSC Adv.*, **2016**, *6*, 73645–73649.

Funding :
Start-up grant, IISER Mohali, DST-SERI (2015-18); DST-INSPIRE (2013-18).

Top left anticlockwise: Sushil, Kavita, Aswathy, Vinita, Prabjot, Narendra.

Jino George
Assistant Professor
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Tel: +91 8146257106

Molecular Strong Coupling Group

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 Coupling Chemistry
Active Plasmonics
Photo-physics 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.

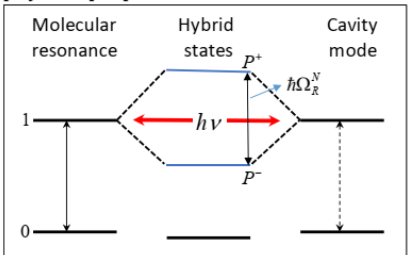

Figure 1: Light-matter hybridization of a cavity and a molecular state.

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.

Project 1: Strong Coupling 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.

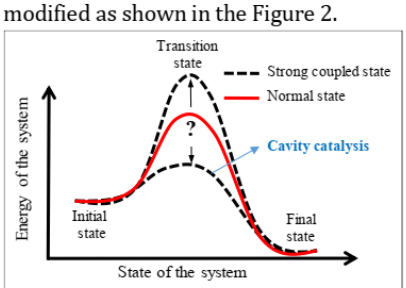

Figure 2: Potential energy surface of a normal one-step reaction (red spectrum) and that of the hypothetical states originated from VSC (black dotted spectrum)

Project 2: Polaritronics

Here, more emphasis will be given for improving the efficiency of 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.

Selected Publications:

(1.) "Ultra-strong coupling of molecular materials: spectroscopy and dynamics" J. George et al., *Faraday Discussions* **2015**, *178*, 281-294.

(2.) "Ground state chemical reactivity under vibrational coupling to the vacuum field" A. Thomas, J. George et al., *Angew. Chem. Int. Ed.* **2016**, *55*, 11462–11466.

(3.) "Conductivity in organic semiconductors hybridized with the vacuum field." E. Orgiu, J. George et al., *Nature Mater.* **2015**, *14*, 1123–1129.

(4.) "Multiple Rabi splitting under ultra-strong vibrational coupling" J. George et al., *Phys. Rev. Lett.* **2016**, *117*, 153601.

(5.) "Tilting a ground-state reactivity landscape by vibrational strong coupling" A. Thomas et.al. *Science* **2019**, *363*, 615-619.

(6.) "Cavity Catalysis by Co-operative Vibrational Strong Coupling of Reactant and Solvent Molecules" J. Lather et.al. *Angew. Chem. Int. Ed.* **2019**, *58, 10635-10638.*

Funding:
DST-SERB-EMR/2017/03455 (2019-21)
STARS-2019/175 (2019-22)

Our websites:
http://www.iisermohali.ac.in/faculty/dcs/jgeorge
https://jinobey.wixsite.com/msc-group

Second row (from left): Pooja, Jaibir, Athul, Thabassum, Akhila and Kuljeet.

First row: Jyoti, Jino and Chithra.

Raj Kumar Roy
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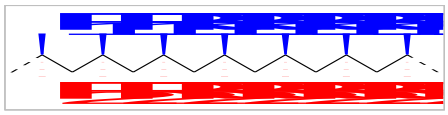
Polymer Chemistry

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.

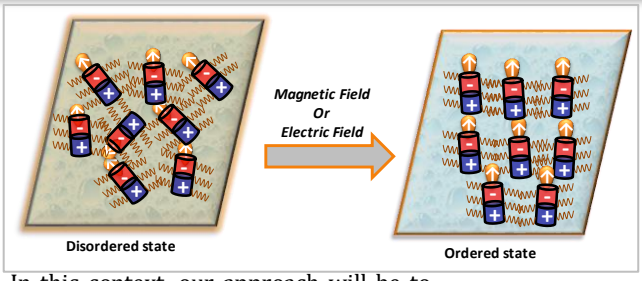


(A) Fundamental investigation on polymerization mechanism and kinetics

In this very broad research area, our group will specifically focus on the development of new organo-catalyst to control the microstructure of the polymer such as tacticity, sequence (primary structure), molecular weight distribution etc, which will allow us to have a deep understanding on structure-property relationship to develop advanced functional material.

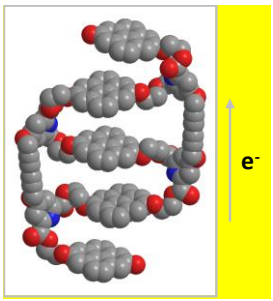
(B) Plastic multiferroic materials

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 leads 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 in a plastic material.

(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 organize π-electron rich moieties by using covalent as well as non-covalent interactions to create charge transport channel across the π-surface.

Left to right: Asha, Raj, Deepak, Ankita, Umer, ShivKumar, Arjun, Subhendu and Arya (missing in this picture).

Selected Publications:

(1) "Design and synthesis of digitally encoded polymers that can be decoded and erased" Roy, R. K.; Meszynska, A.; Laure, C.; Charles, L.; Verchin, C.; Lutz, J.F. *Nat. Commun.* **2015**, *6*, 7237.

(2) "Compartmentalization of single polymer chains by stepwise intramolecular crosslinking of sequence-controlled macromolecules" Roy, R. K.; Lutz, J.F. *J. Am. Chem. Soc.* **2014**, *136*, 12888-12891. (Highlighted in ***Nature Nanotechnology*** doi:10.1038/nnano. **2014**.239 & ***JACS* spotlight**.

(3) "Convergent synthesis of digitally encoded poly (alkoxyamine amide) s" Roy, R. K.; Laure, C.; Fischer Krauser, D.; Charles, L.; Lutz, J.F. *Chem. Commun.* **2015**, *51*, 15677-15680.

(4) "Periodically Grafted Amphiphilic Copolymers: Nonionic Analogues of Ionenes" Roy, R. K.; Gowd, E. B.; Ramakrishnan, S. *Macromolecules* **2012**, *45*, 3063-3069.

(5) "Control of Molecular Weight and Polydispersity of Hyperbranched Polymers Using a Reactive B3 Core: A Single-Step Route to Orthogonally Functionalizable Hyperbranched Polymers" Roy, R. K.; Ramakrishnan, S, *Macromolecules* **2011**, *44*, 8398-8406.

Funding:

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

Subhabrata Maiti
Assistant Professor
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Tel: +91-9836553791

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 –

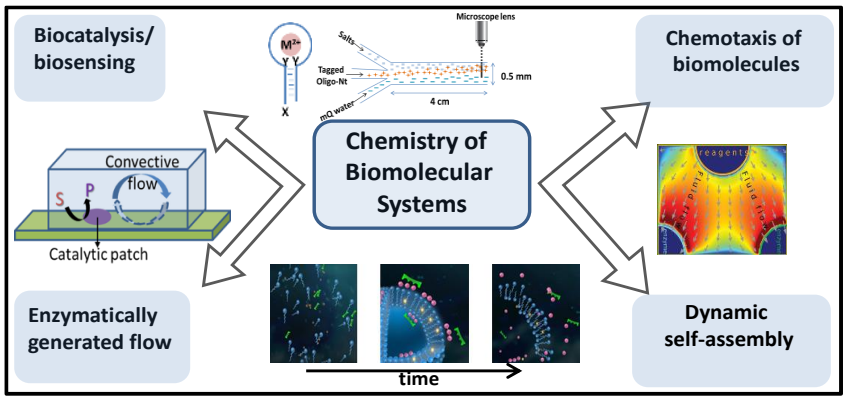
Dynamic self-assembly: In this context it is worthy to mention that one of the fundamental feature of life is that it operates out-of-equilibrium and it needs constant influx of energy to remain in a dynamic state. This inspires us to develop synthetic system (involving enzymes) which are chemical fuel-responsive 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/mysite



Selected Publications

(1) "Sucrose-mediated heat-stiffening microemulsion-based gel for enzyme entrapment and catalysis" Akshi Deshwal, Himanshu Chitra, Madhusudan Maity, Santanu K Pal, Subhabrata Maiti* ***Chem. Commun.*** **2020,** DOI:10.1039/D0CC04294C.

(2) "Deconvolution of Transient Species in a Multivalent fuel - driven Multistep Assembly under Dissipative Condition" Ekta Shandilya, Subhabrata Maiti*. ***ChemSystemsChem***, **2020**, *2*, e1900040.

(3) "Self-organization of fluids in a multi-enzymatic pump system" Subhabrata Maiti, Oleg Shkylev, Anna Balazs and Ayusman Sen, ***Langmuir*** **2019**, 35, 3724. (cover page)

(4) "Fuel-Selective Transient Activation of Nanosystems for Signal Generation" Flavio della Sala, Subhabrata Maiti, Andrea Bonanni, Paolo Scrimin and Leonard J. Prins. ***Angew. Chem. Int. Ed.*** **2018**, 57, 1611.

(5) "Dissipative self-assembly of vesicular nanoreactors" Subhabrata Maiti, Ilaria Fortunati, Camilla Ferrante, Paolo Scrimin and Leonard J. Prins, ***Nature Chemistry***, **2016**, 8, 725.

(6) "Multivalent interactions regulate signal transduction in a self-assembled Hg^{2+} sensor", Subhabrata Maiti, Cristian Pezzato, Sergio Garcia Martin and Leonard J. Prins, ***J. Am. Chem. Soc.***, **2014**, 136, 11288.

Group members: (From left to right) Himanshu, Basundhara, Ekta, Dr. Maiti, Sheetal, Priyanka, Akshi

Monika Sharma
INSPIRE Faculty
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Computational Biophysical Chemistry

Profile:

Inspire Faculty – 04, 2015 – Current /IISER,Mohali
Ph.D – 2007-12/IIIT,Hyderabad/Prof. Abhijit Mitra and Prof. Harjinder Singh
Postdoc – 2012-13/Michigan State University/USA/Prof. Michael Feig
- 2013-14/NINDS-NIH/USA/ Dr. Lucy Forrest
Others – DAAD Fellow/04-10,2010/Max Planck Institute of Biophysical Chemistry /Goettingen/Germany

Research Interests:

I am interested in application of computational methods to study the conformational dynamics of the biomolecules and interactions among them. I primarily uses molecular dynamics and molecular modelling as principal tools for the theoretical study of biological molecules and their complexes. These simulation techniques include conventional MD simulations and enhanced simulation methods such as umbrella sampling, replica exchange MD, free energy perturbation, targeted MD, and steered MD.

Computer Aided Drug Designing or Protein Designing

These ongoing projects with experimental labs involved protein modeling in conjunction with docking of ligands or drug molecules are being used to understand their interactions or to suggest structure-guided mutagenesis.

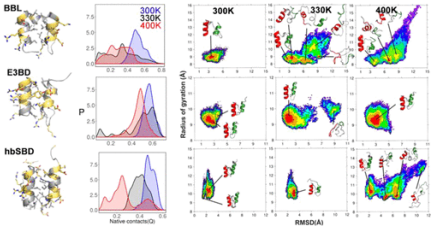
- Structure-guided mutagenesis of sugar acid metabolism regulators
- Design of HDAC Class-I family inhibitors as probable epigenetic regulators
- Role of pathogenic SNPs in structural stability of BLM helicases.
- Molecular docking for design and synthesis of sulfur cross-linked 1,3,4-oxadiazole-nitro(furan/thiophene) propenones as dual inhibitors of inflammation and tuberculosis.

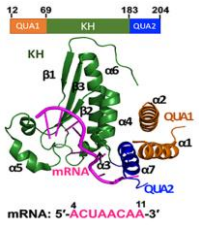
***In silico* studies to understand RNA complexation by STAR proteins**

Signal Transducer and Activator of RNA (STAR) proteins, such as mammalian QKI, metazoan GLD-1, or SF1 have been shown to function in pre-mRNA splicing, mRNA export, mRNA stability, and protein translation. These have critical implications in many cellular processes. and reported to be associated with numerous human pathologies like cancers and neurological disorders such as human inherited ataxia, multiple sclerosis, or schizophrenia. Combining unbiased simulations with essential dynamics and network analysis, we investigated how presence of mRNA affects stability, dynamics, and allosteric communication within STAR domain. This work was extended to understand the binding specificities of target mRNA sequences by human QKI protein.

Investigating protein folding using unfolding dynamics

Capturing the events during denaturation pathways is crucial for understanding various aspects such as, loss of enzymatic and biological activities of proteins at higher temperatures or in presence of chemicals, which is of utmost importance for biotechnological applications. MD simulations of the unfolding of three peripheral subunit binding domains sharing similar folds showed cooperative unfolding transitions of these proteins.





QKI protein with bound mRNA (in pink)

Modeling of transporters

This project involves modeling of transporters to understand the molecular basis of their substrate binding and specificity. In collaboration with experimentalists, theoretical modeling of two fungal transporters proteins: (a) high affinity glutathione binding, Hgt1p and (b) cystine transporter, CgCYN1 was mapped with the experimental mutagenesis. Another work on transporter involves unravelling the substrate efflux-influx of human cystine-glutamate antiporter, xCT, and modeling in different conformational states.

Selected Publications:

(1) "Unfolding Transitions of Peripheral Subunit Binding Domains show Cooperative Behavior". M. Sharma, G. Bulusu and A. Mitra **2019**. *J Phys Chem B*. 123(16):3441-3451.

(2)"Interpretation of spectroscopic data using molecular simulations for the secondary active transporter BetP" V. Leone, I. Waclawska, K. Kossmann, C. Koshy, M. Sharma, T.F. Prisner, C. Ziegler, B. Endeward, L.R. Forrest **2019.** *J. Gen Physiol*. 151(3):381-394.

(3)"Mechanism of mRNA-STAR domain interaction: Molecular dynamics simulations of Mammalian Quaking STAR protein". M. Sharma and C.R. Anirudh **2017.** *Scientific Reports*. 7: 12567.

(4)"Insights into the molecular basis for substrate binding and specificity of the fungal cystine transporter CgCYN1." A.A. Deshpande, M. Sharma and A.K. Bacchawat **2017**. *BBA-Biomembranes*. 1859(11): 2259-2268.

(5)"Substrate specificity and mapping of residues critical for transport in the high-affinity glutathione transporter Hgt1p" M. Zulkifli, S.Yadav, A.Thakur, S.Singla, M. Sharma, and A.K.Bachhawat. 2016. *Biochem J.* 473(15):2369-2382

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Inspire Faculty
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Tel: +91 7744029918

Chemistry at Nanoscale

Profile:

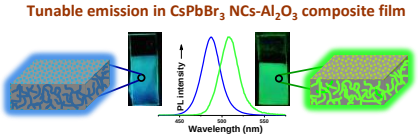
Ph.D – 2007-12/Jadavpur University (CSIR-Central Glass & Ceramic Research Institute), Kolkata, India/Dr. Goutam De
Postdoc – 2013-15/University of Cincinnati, Ohio, USA /Dr. Laura Sagle
Postdoc – 2015-16/IISER-Pune, Pune, India /Dr. G. V. Pavan Kumar
Professional experience – 2016-present/INSPIRE Faculty/IISER Mohali, Mohali, India

Research Interests:

Our 'Chemistry at nanoscale' group is interdisciplinary in nature. Group's research work mainly consists of synthesis of materials in nanoscale, understanding their property, application study and lab scale device fabrication. Research directions are given below:

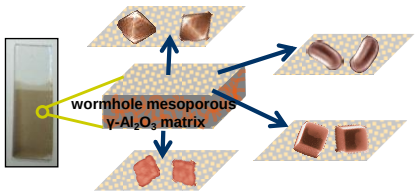
Perovskite nanocrystals:

We are investigating a new pathway towards generation of stable perovskite nanocrystals (Pb based) in mesoporous thin film. This protocol has shown significant improvement regarding stability of perovskites and also the whole process can be done at room temperature and ambient atmosphere. These coatings on glass as well as flexible plastic substrates would be useful in LED, backlit displays. In the next step, to overcome the toxicity issues of Pb, development of non Pb based perovskite nanocrystals will be undertaken and their potentiality towards optoelectronic and photovoltaic applications will be evaluated.



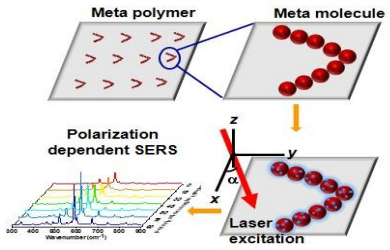
Mesoporous materials and nanocomposites:

Nanoscale structural proficiencies and high surface area in mesoporous materials combined with fascinating properties of metal nanoparticles make the nanocomposites suitable candidate towards adsorption, separation, drug delivery, sensors, catalysis, energy storage and conversion. In this context, we are interested in fabricating hybrid mesoporous oxides with ordered mesopores having different symmetrical pore arrangement by cooperative assembly as well as liquid crystal templating approach. The next challenge is to incorporate/generate metal nanoparticle, graphene dot, semiconductor quantum dots etc. inside the mesoporous channel keeping in view the goal to fabricate advanced materials for optoelectronic, catalytic applications.



Estimation of optical enhancing properties of nanoparticle assemblies and coupled nanostructures:

Surface enhanced Raman spectroscopy is capable of probing single molecule and plasmonic nanoparticles are required to provide the electromagnetic field needed for this enhancement. This enhancement can be tailored by the shape, size and composition as well as the extent of coupling between the nanoparticles. We would like to examine the effect on SERS enhancement by different shaped coupled nanostructures and nanoparticle assemblies.



Selected Publications:

(1)"Stable Mn-Doped CsPbCl3 Nanocrystals inside Mesoporous Alumina Films for Display and Catalytic Applications" Antony K.J., I.; Jana, D. *ACS Appl. Nano Mater.*, **2020**, DOI: 10.1021/acsanm.0c00213.
(2) "Room temperature synthesis of blue and green emitting $CsPbBr_3$ perovskite nanocrystals confined in mesoporous alumina film" Takhellambam, D.; Meena, T. R.; Jana, D.* *Chem. Commun.*, **2019**, 55, 4785–4788.
(3) "V-shaped active plasmonic meta-polymers" Jana, D.* Vasista, A. B.; Jog, H.; Tripathi, R. P. N.; Allen, M.; Allen, J.; Pavan Kumar, G. V. *Nanoscale,* **2019**, 11, 3799–3803.
(4) "How Does "Wormhole" Mesoporous γ-Alumina Matrix Direct the Morphology of Pt Nanocrystals?" Jana, D.*; De, G. *Cryst. Growth Des.* **2019**, 19, 1494–1501.
(5) "Surface Enhanced Raman spectroscopy of a Au@Au core-shell structure containing a spiky shell" Jana, D., Gorunmez, Z., He, J., Bruzas, I., Beck, T., Sagle, L., *J. Phys. Chem. C,* **2016**, 120, 20814–20821.

Group members: (From left) Megha, Ashitha, Dr. Debrina, Dhanvin

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Tel: +91 9779144905

Theoretical/Computational Chemistry

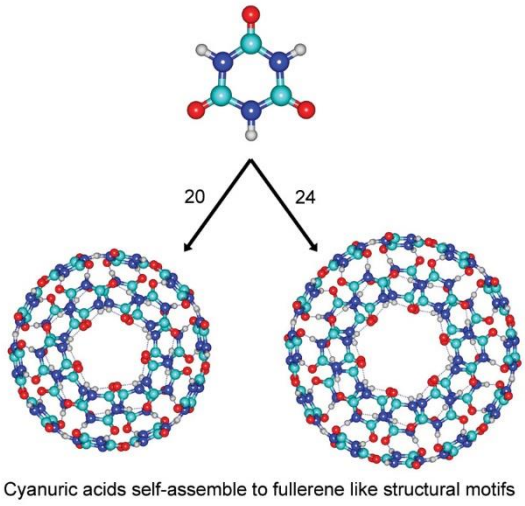
Profile:

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- IIT Kanpur; 2007- IISER Mohali

Research Interests:

Professor Sathyamurthy's research interest has been investigations in the area of molecular reaction dynamics, using quasiclassical trajectory calculations and time-dependent quantum mechanical methods as tools. Starting from ab initio calculations of the potential energy surface and fitting an analytic function to the ab initio data and using the potential energy surface to compute state-to-state reaction cross section and other observables for elementary chemical reactions has been the major activity of the group. The group had focused special attention on the dynamics of He + $H_2^+ \rightarrow HeH^+ + H$ reaction and the isotopic branching in He, HD^+ collisions. Recently, they have reported the results of a three dimensional quantum mechanical study of the collision induced dissociation process too. In all cases, the computed results have been compared with the best available experimental results. Perhaps, one of the best ab initio potential energy surfaces for the H_3-system comes from the group.

More recently, Sathyamurthy and his students have been investigating the structure and stability of water clusters, boric acid clusters, endohedral fullerenes, and gas hydrates. The role of structural motifs in deciding the shapes of clusters has been the focus of attention. The results on gas hydrates have significant practical application too.



Cyanuric acids self-assemble to fullerene like structural motifs

Determining accurate ab initio potential energy curves for the ground and excited states of anionic species is a challenging task. This is particularly so because of the curve crossing between the anionic and neutral species and the resulting autoionization. The group has computed reliable ab initio potential energy curves for H_2^-, CH^-, NH^- and OH^-. They have paid special attention to the study of the ground and excited electronic states of isoelectronic species to understand the relation between the neutral and the anionic species.

With the help of highly accurate ab initio potential energy curves for the ground and excited states of CO, the group has computed the absorption spectrum and also predicted the spectral features arising from indirect predissociation in CO.

6-prismane: $[C_nSi_{(6-n)}H_6]_2$
$n\uparrow$ stability$\downarrow$

Selected Publications:

(1) Nanoclusters of Cyanuric Acid, M. Elango, V. Subramanian and N. Sathyamurthy, *J. Chem. Sci.* (Special issue in honor of Charusita Chakravarty) **2017,** 129, 873-881.

(2) Stabilisation of the [6]-prismane structure by silicon substitution, A. Equbal, S. Srinivasan and N. Sathyamurthy, *J. Chem. Sci.* (Special issue in honor of Charusita Chakravarty) **2017**, 129, 911-917.

(3) A study of topological effects concerning the lowest A" and the three A' states for the CO_2^+ ion , V. Dhindhwal, M. Baer, N. Sathyamurthy, *J. Phys. Chem. A* **2016**, 120, 2999.

(4) Interpretation of the accidental predissociation of the $E^1\Pi$ state of CO, M. Majumder, N. Sathyamurthy, G. J. Vazquez, H. Lefebvre-Brion, *J. Chem. Phys.*, **2014**, 140, 164303.

(5) Ab initio potential energy curves for the ground and low lying excited states and the effect of $^2\Sigma^\pm$ states on Λ-doubling of the ground state X $^2\Pi$ of NH^- S. Srivastava and N. Sathyamurthy, *J. Phys. Chem. A*, **2013**, 117, 8623–8631.

Ramesh Kapoor
Professor (Retired)
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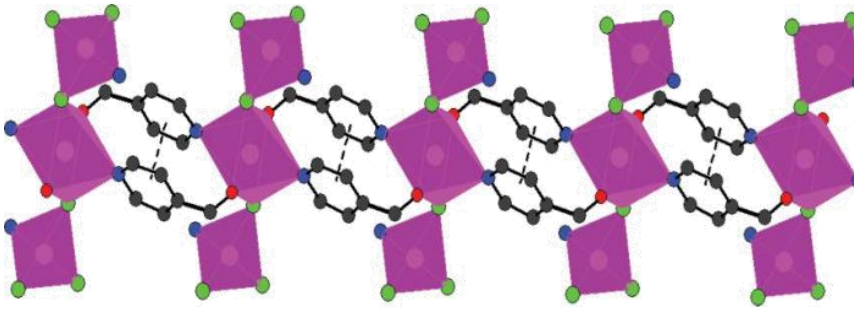
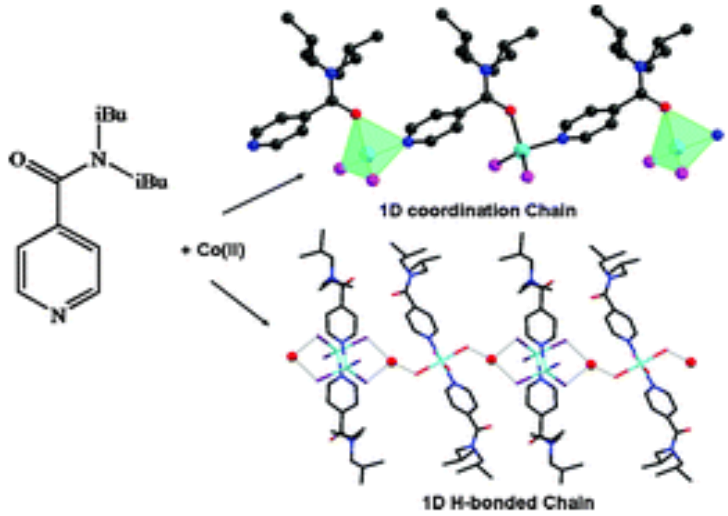
Inorganic and Coordination Chemistry





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 coordinatioon geometrics 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.

K. S. Viswanathan
Professor (Retired)
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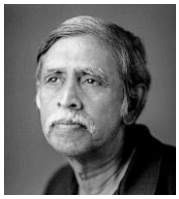
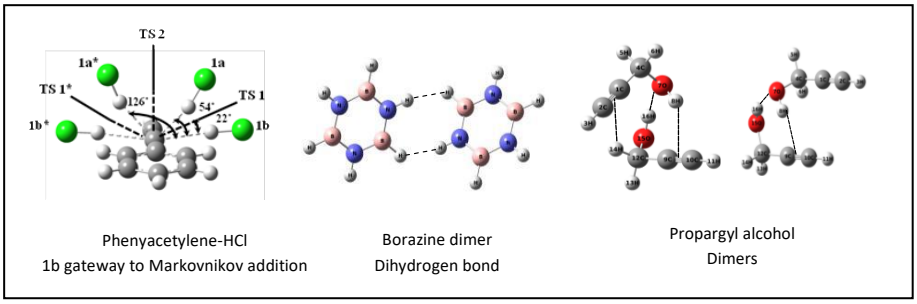
Tel: +91 9530802088



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



Phenyacetylene-HCl
1b gateway to Markovnikov addition

Borazine dimer
Dihydrogen bond

Propargyl alcohol
Dimers

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 N_2, for eventual study by infrared spectroscopy. Using this technique, non-covalent interactions and molecular conformations are studied.

Group (Past & Present): 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: 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-C_2H_2 dimer from the C_6H_6-C_2H_2 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

From Left: Pankaj, Priyanka, Jyoti, Amala, Anamika, Kanupriya, Vish, Ginny, Divita.

Bimalendu Adhikari
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Tel: +91 9933898711

Molecules to Materials

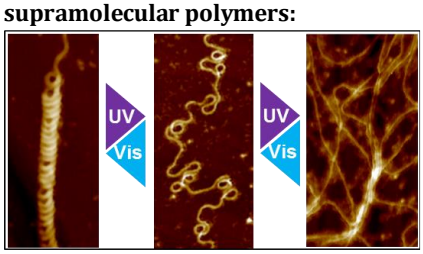
Profile:

Ph.D – 2007-2012/ Indian Association for the Cultivation of Science, Kolkata, India / Prof. Arindam Banerjee
Postdoc – 2012-2015/University of Toronto, Toronto, Canada /Prof. Heinz-Bernhard Kraatz
Postdoc– 2015-2016/Chiba University, Chiba, Japan/JSPS Fellow/Prof. Shiki Yagai
Professional experience – 2016-present/ INSPIRE Faculty/IISER Mohali, Mohali, India

Research Interests:

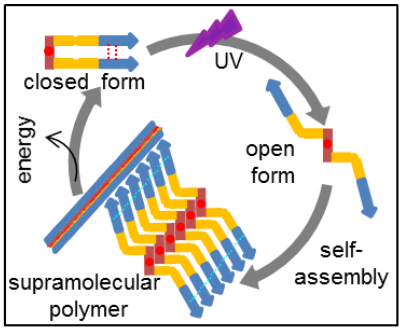
Supramolecular Polymer, Dissipative and Non-dissipative Assemblies, Gels, Bioorganic Chemistry, Peptides, Nanomaterials

Biology-inspired non-equilibrated supramolecular polymers:



Kinetically controlled non-equilibrium systems have recently attracted great attention due to their diverse functional potential in biological aspects. The strategy for devising robust yet adaptive materials could be possible by using strong noncovalent forces for making non-equilibrated supramolecular polymers (SPs). With this notion we have recently designed molecular systems that could form stimuli-responsive yet robust SPs with diverse structures, depending on their pathway of preparation.
Funding: DST-INSPIRE (ongoing, 2016-till date)
Contributors: Aleena Thomas (Graduate

Light-powered dissipative self-assemblies:



In devising dissipative far-from-equilibrated SPs with high turnover number of recyclability an azobenzene moiety is proposed to exploit light as a source of energy. The noninvasive nature of light would help in proceeding the reversible process in a cyclic manner with high turnover number. An unprecedented level of light-powered far-from-equilibrated SP with dynamic instability (as an active material) would be harnessed, which may ultimately show emergent properties analogous to biological system.
Funding: Submitted to DST-ECR
Contributors: Sujeesh P. T., Joyal Davis (Master students)

Biomolecule based functional gels and smart nanomaterials: Short peptides, nucleosides, and DNA (for instance polyadenine) based responsive soft materials are being developed for bio-applications.

From left to right: Joyal, Bimalendu, Sujeesh, Geethu and Aleena

Funding: DST-INSPIRE (ongoing, 2016-till date)
Contributors: Aleena Thomas (Graduate student), Geethu Venugopal, Joyal Davis (Master students)

Selected Publications:

(1) "Light-Induced Unfolding and Refolding of Supramolecular Polymer Nanofibres" Adhikari, B.; Yamada, Y.; Yamauchi, M.; Wakita, K.; Lin, X.; Aratsu, K.; Ohba, T.; Karatsu, T.; Hollamby, M.; shimizu, N.; Takagi, H.; Haruki, R.; Adachi, S.; Yagai, S., *Nat. Commun.*, **2017**, 8, 15254.
(2) "Hydrogen-Bonded Rosettes Comprising π-Conjugated Systems as Building Blocks for Functional One-Dimensional Assemblies" Adhikari, B.; Lin, X.; Yamauchi, M.; Ouchi, H.; Aratsu, K.; Yagai, S., *Chem. Commun.*, **2017**, doi: 10.1039/C7CC04172A.
(3) "Amino Acid Chirality and Ferrocene Conformation Guided Self-Assembly and Gelation of Ferrocene–Peptide Conjugates" Adhikari, B.; Singh, C.; Shah, A.; Lough, A. J.; Kraatz, H.-B., *Chem.–Eur. J.*, **2015**, 21, 11560.
(4) "A Gel Based Novel Trihybrid System Containing Nanofibers, Nanosheets and Nanoparticles: Modulation of Rheological Property and Catalysis" Nanda, J.; Biswas, A.; Adhikari, B.; Banerjee, A., *Angew. Chem., Int. Ed.*, **2013**, 52, 5041.
(5) "Pyrene-Containing Peptide-Based Fluorescent Organogels: Inclusion of Graphene into the Organogel" Adhikari, B.; Nanda, J.; Banerjee, A., *Chem.–Eur. J.*, **2011**, 17, 11488.
(6) "Facile Synthesis of Water-Soluble Fluorescent Silver Nanoclusters and Hg^{II} Sensing" Adhikari, B.; Banerjee, A., *Chem. Mater.*, **2010**, 22, 4364.

Visiting Faculty

Dr. J. Narasimha Moorthy

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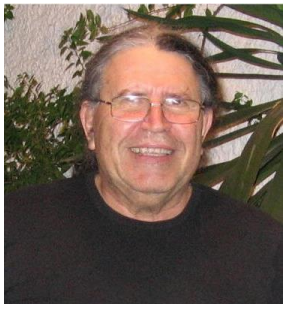
E- mail: rmohan@iwu.edu
Telephone: +1 309-556 3829
Period: October – December 2012, October 2015, August 2016 & August 2017
Course taught: Green Chemistry



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
E- mail: mangal@iitm.ac.in
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

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 were 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. Shamasunder (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 chemicalsput 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. Arulananda 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.

Organizing Secretary and Chairman: Dr. S. A. Babu, Department of Chemical Sciences, IISER 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.

Courses offered by the Department

BS-MS Programme Courses for Core Semesters (1st and 2nd year)

Course Number	Title	Credits
CHM101	Chemistry of elements and chemical transformations	3
CHM111	Chemistry Lab I	1
CHM102	Atoms molecules and symmetry	3
CHM112	Chemistry Lab II	1
CHM201	Spectroscopic and other physical methods	3
CHM211	Chemistry Lab III	1
CHM202	Energetics and dynamics of chemical reactions	3
CHM212	Chemistry Lab IV	1

BS-MS Programme Courses for Chemistry Majors (3rd year)

CHM301	Quantum Chemistry	4
CHM302	Organic Reactions	4
CHM303	Main group chemistry	4
CHM311	Organic chemistry lab	4
IDC351	Seminar (Attending)	1
******	Open Elective I	4
CHM304	Symmetry in chemistry	4
CHM305	Physical organic chemistry	4
CHM306	Transition metal chemistry	4
CHM312	Inorganic chemistry lab	4
******	Open Elective II	4
IDC305	Selected Analytical Techniques	4
IDC352	Seminar (Attending)	1

BS-MS Programme Courses for Chemistry Majors (4th year)

CHM401	Molecular spectroscopy	4
CHM402	Chemistry of materials	4
CHM411	Physical chemistry lab	4
CHM***	Chemistry Elective I	4
******	Open Elective III	4
IDC451	Seminar (Delivering)	1
CHM403	Analytical chemistry	4
CHM404	Statistical thermodynamics	4
CHM412	Analytical chemistry lab	4
CHM***	Chemistry Elective II	4
******	Open Elective IV	4
IDC452	Seminar (Delivering)	1

Courses offered by the Department

Elective and PhD Courses

Course Number	Title	Credits
CHM307	Electrochemistry and ionic equilibria	4
CHM601	Advanced inorganic chemistry	4
CHM602	Magnetic resonance	4
CHM603	Elements of NMR theory	4
CHM604	Advanced organic chemistry	4
CHM605	Advances in solid state NMR	4
CHM606	Bio-organic 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	Computational chemistry	4
CHM617	Chemical dynamics and non-adiabatic interactions	4
CHM618	Bioinorganic chemistry	4
CHM619	Numerical methods in chemistry	4
CHM620	Energetics and dynamics of chemical reactions – 2	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
CHM625	Molecular Dynamics Simulations	4
CHM626	Photochemistry – concepts, techniques and applications	4

Research 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
- Jeol Tunneling Electron Microscope

Departmental Research Lab Facilities

- 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

- LABINDIA AA7000 Atomic Absorption Spectrophotometer (1 No)
- LABINDIA UV-Vis Spectrophotometer (6 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: Intel(R) Xeon(R) CPU X5670 @ 2.93GHz with a total of over 288 processor cores ,Head Node + 24 Nodes + Workstation

Alumni Placements

Name	Batch	Current/Past Position
Mrinal Shekhar	MS07	PhD at University of Illinois at Urbana–Champaign. Post-doc at Broad Institute of MIT and Harvard, USA.
Shalender Jain	MS07	Lecturer at Govt. College Haryana.
Gaurav Kumar	MS08	PhD at University of Southern California, USA. Currently Post-doc at Photon Science, Stanford Pulse Institute, USA.
Kapil Dave	MS08	PhD at University of Illinois, Urbana-Champaign, USA. Currently R&D Engineer, Intel Corporation, USA.
Asif Iqbal	MS08	PhD at Aarhus university, Denmark and TIFR Mumbai. Post-doc at Univ. California, Santa Barbara.
Vinod Kumar	MS08	PhD at IISER Mohali.
Sumit Mittal	MS08	Assistant Prof. at VIT Bhopal
Deepansh Shrivastava	MS08	PhD at Ohio State university, USA.
Manish Pareek	MS08	Senior Scientist, Signature Discovery Ltd, UK.
Mariyam Fatima	MS09	PhD at Max Planck Institute of Structure and Dynamics of Materials, Germany. Currently Post-doc fellow at DESY, Hamburg, 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 Jhajharia	MS09	PhD at École Normale Supérieure, Paris.
Gaurav Verma	MS09	PhD at University of South Florida, USA (PhD completed in 2020).
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.
Vikash Dhindhwal	MS09	Civil Service.
D. Jeiyendira 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 student at Technische Universität München, Germany.
Ravi Ranjan	MS10	PhD student at NCL Pune.
Bharti Kumari	MS10	PhD at Technische Universität Darmstadt, Germany.
Piyush Mishra	MS10	PhD at Purdue University, USA. Currently Post-doc fellow at MIT, Boston, USA.
Pratip Chakraborty	MS10	PhD at Temple University, USA.
Jagadish Prasad Hazra	MS10	PhD at IISER Mohali.
Ashish Kumar	MS10	PhD at IISER Mohali.
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	PhD at IISER Mohali.
Haseeb Hakkim	MS10	PhD at IISER Mohali.
Arya J. S	MS10	PhD at CSIR - NIIST, Kerala.
Raut Akshay Hemant	MS10	PhD at Ruhr University of Bochum, Germany. Currently Post-doc fellow at ETH, Zurich.

Alumni Placements

Rupali Chawla	MS10	PhD student at Ruttgers 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 student at University of Quebec at Trois-Rivieres, Canada.
Akhil V. Gopal	MS10	PhD student at IISER Kolkata.
Ankit Kumar Agrawal	MS10	PhD student at CSIR-IIP, Dehradun.
Soniya Rani	MS10	PhD student at NCL Pune.
Nitish Kumar	MS10	Preparing for IAS and Bank Exams.
Nitin Kumar Singh	MS10	PhD at IISER Mohali, India.
Shweta Sreenivasan	MS11	Ph. D. at Massachusetts Institute of Technology.
Nakul Thete	MS11	Ph. D. at Virginia Tech, Virginia.
Srijit Mukherjee	MS11	Ph. D. at University of Colorado, Boulder.
Justin K. Thomas	MS11	Ph. D. at Ohio state University, Columbus.
Lakshmi Bhai N. V.	MS11	Ph. D. at Ohio state University, Columbus.
Manisha	MS11	Ph. D. student, Massachussets University, Amherst.
Jopaul Mathew	MS11	Ph. D. student, Virginia Tech.
Sabari	MS11	N.A.
Abhinay Vardhan	MS11	Ph. D. at IISER Mohali.
Sandhya Singh	MS11	Ph. D. student, University of Otago, New Zealand.
Anjali Mahadevan	MS11	Ph. D. at IISER Mohali.
Athira T. John	MS11	Ph. D. at IISER Trivandrum.
Sruthi Mohan	MS11	Ph. D. Student, 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	Institute of Energy and Climate Research, Julich, Germany.
Aman Kumar Bhonsle	MS11	Ph. D. Student, Indian Institute of Petroleum, Dehradun.
Neeru Mittal	MS12	Ph. D at ETH Zurich.
Aayush	MS12	Ph. D at Purdue University.
Satavisa Jana	MS12	Ph. D at UCSD, California San Diego.
Bhupendra Goswami	MS12	Ph. D at Karlsruhe institute of Technology, Germany.
Ankit	MS12	Ph. D. at IISER Mohali.
Aleena Anna Thomas	MS12	Ph. D. at IFW, Dresdan Germany.
Mushir Ul Hassan	MS12	Ph. D. at Temple University.
Anuj Pennathur	MS12	Ph. D. at University of Southern California.
Anirudh CR	MS12	Ph. D. at Michigan State University.
Mustafa Iqbal	MS12	Ph. D. at TU Vienna, Austria.
Ravi Ranjan	MS12	Ph. D. at University of Illinois, Chicago.
Mohammed Shabin	MS12	Project assistant, IISER M.
Sruthy Chandy	MS12	Ph. D. at Indiana University, Bloomington.
Ajit Kumar Yadav	MS12	Kota Institute.
Dr. Manish Pareek	MS12	Post-doc at Paris-Sud University, France.
Siddhant V. Wagulde	MS12	Ph.D. student, University of Texas, Dallas.
Neeru Mittal	MS12	PhD, ETH Zurich.

Alumni Placements

Anuj K Pennathur	MS12	PhD student, University of Southern California, USA.
Nimya SS	MS12	PhD student, Indian Institute of Tropical Meteorology, Pune.
Vikram Singh Bhati	MS12	ALLEN Career institute, Kota.
Sumit Kumar Agarwal	MS12	PhD student, BITS, Pilani.
Ebin George	MS12	Assistant Manager, SBI.
Bharti Sohpaul	MS12	Team Lead and SME- Chemistry, Evelyn Learning Systems Pvt. Ltd.
Shreyan Ganguly	MS13	Ph. D. at IISER Mohali.
Virender Singh	MS13	PhD, IOCB, Prague (offered).
Ankit Somani	MS13	PhD, Ruhr University Bochum, Germany.
Lisha Loitongbam	MS13	N.A.
Vaishnavi Sidharthan	MS13	PhD student at the Ohio State University, USA.
Nitya Singh	MS13	N.A.
Neelima P R	MS13	M. Phil student at CUSAT Kochi, India.
Swathy Lekshmy V S	MS13	N.A.
Mr. Chaman Lal Mahawar	MS13	Inspector, Central Board of Excise and Customs (CBEC), Kolkata.
Saurabh Mhatre	MS13	Ph. D. Student, FSU Jena, Germany.
Anuj Kumar	MS13	Ph. D student in TU, Delft.
Meghanad Kayanattil	MS13	PhD student, Max Planck Institute (Hamburg, Germany).
Pragya Verma	MS13	PhD student, University of Geneva, Switzerland.
Divita Gupta	MS13	PhD at Universite de Rennes, France.
Priyanka Bansal	MS13	PhD at EPFL, Switzerland .
Amala Raj	MS13	PhD at Indiana University, USA.
Omprakash	MS13	Faculty, Allen Institute, Chennai.
Ajit Kumar Yadav	MS13	Faculty, Allen Institute.
Siddharth K Kurdia	MS13	MBA, IBS, Mumbai.
Daimiota Takhellambam	MS14	PhD at University of Rome, Italy (Centre for Hybrid and Organic Solar energy).
Irin P. Tom	MS14	PhD, University of Illinois at Chicago (offered).
Amal Sam Sunny	MS14	PhD, University of Miami, USA.
Vaitheesh J	MS14	PhD, University of Miami, USA.
Virinder Bhagat	MS14	PhD, University of Tuebingen, Germany.
Amandeep Singh	MS14	Ph. D. at IISER Mohali.
Divanshu Gupta	MS14	PhD, 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 B C	MS14	Going for PhD at Indiana University.
Mythreyi R. M	MS14	Ph. D. student, University of Southern California.
Vishal Tiwari	MS14	Ph. D. student, University of Rochester.
Rishabh Gupta	MS14	Ph. D. student, Purdue University.
Shruthi S. Nair	MS14	Ph.D. student, Friedrich Schiller Universitat Jena, Germany.
Suresh Kumar	MS14	Ph.D. student, Friedrich Schiller Universitat Jena, Germany.
Lejjish V P	MS14	Ph.D. student, University of Eastern Finland, Finland.
Pinku Tung	MS14	Ph.D. student, University of Illinois, Chicago, USA.
Shivangi Kharbanda	MS14	Ph.D. student, Oklahoma State University, OK, USA.
Nikam Mrudula Mangesh	MS14	Ph.D. student, TIFR Hyderabad (to be joining)
Animesh Singh	MS14	Preparing for UPSC.

Alumni Placements

Rishab Gupta	MS14	Ph.D. student, Purdue University, West Lafayette, USA.
Abdul Haseeb M.M.	MS14	Ph.D. student, University of Illinois , Chicago, USA.
Md Misbahur Rehman	MS14	Ph.D. student, King Abdullah University of Science and Technology, UAE.
Vishal Porwal	MS14	Ph.D. student, University of Lorraine, France (offered).
Himanshi Singh	MS14	Ph.D. student, Deutsche Elecktron Synchrotron , Hamburg, Germany.
Ajeet Kumar	MS14	Ph.D. student, Technical University of Munich, Germany.
Kripa Joseph	MS14	Ph.D. student, University of Strasbourg, Strasbourg, France.
Vidhya Lakshmi	MS14	Ph.D. student, The Ohio State University, USA.
Jai Khatri	MS14	Ph.D. student, Ruhr University, Bochum, Germany.
Diksha Sharma	MS14	MBA student, XLRI, Jamshedpur, India.
Parth Raval	MS14	Ph.D. student, University of Lille, Lille, France.
Lejjish V P	MS14	Ph.D. student, University of Eastern Finland, Finland.
Isabella Antony	MS14	Project Assistant, IISER Mohali.
Nihal P C	MS14	College Lecturer.
Nitish Kumar Garg	MS14	PhD at University of Lund, Sweden.
Shivangi Vaish	MS14	Ph. D. Indiana University, Bloomington, Indiana, USA (offered).
Dipali Singh	MS14	Ph. D. at Univ. of Hamburg, Germany (offered).
Asha Ramesh	MS14	PhD at IIT Hyderabad (Yet to join)
Arya Ajith	MS14	Project Assistant at MG university, Kerala.
Kaustav Chatterjee	MP15	PhD at Indiana University, USA.
Pankaj Seliya	MP16	Ph.D. student, Max Planck Institute for Polymer Research, Germany.
Soumyadeep Chakravorty	MP16	Ph.D. student, University of Rostock, Germany.
Kaushalendra Patel	MP16	Ph.D. student, IISER Mohali.

Ph. D Students

Name	**Year**	**(Ph. D Supervisor) and Current/past Position**
Dr. Sadhika Khullar	2013	(Prof. Sanjay Mandal), Assistant Professor, NIT Jalandhar.
Dr. Neha Jain (Bio PhD)	2013	(Dr. Samrat Mukhopadhyay), Assistant Professor, IIT Jodhpur.
Dr. Zeba Qadri	2014	(Dr. R. Ramachandran), Post-doc at Harvard Medical School, Boston.
Dr. Shruti Arya	2015	(Dr. Samrat Mukhopadhyay) Post-doc at Univ. of California Santa Barbara, USA.
Dr. Dominic Narang	2015	(Dr. Samrat Mukhopadhyay), Post-doc at University of California San Diego, USA.
Dr. Vijit Dalal	2015	(Dr. Samrat Mukhopadhyay), Scientist, Benitec Inc. San Francisco Bay Area, USA.
Dr. Gurpreet Kaur	2015	(Dr. Angshuman Roy Choudhury), Assistant Professor, DAV University, Jalandhar (2016-2018), currently Post-doc research associate at the Hebrew University, Jerusalem since 2018.
Dr. Navnita Kumar	2015	(Prof. Sanjay Mandal), Post-doc: University of California, Los Angeles.
Dr. Billa Prasanth	2015	(Dr. Sanjay Singh), Post-doc at University of Bonn.
Dr. R. Venkata Subba Rao	2016	(Dr. Ramesh Ramachandran), Post-doc : TCIS, Hyderabad.
Dr. U. Sivaranjan	2016	(Dr. Ramesh Ramachandran), Post-doc: Hebrew University.
Dr. Seema Rani	2016	(Dr. S. S. V. Ramasastry), Marie-Curie postdoctoral fellow, Friedrich Schiller University Jena, Germany.
Dr. Nayyar Ahmad Aslam	2016	(Dr. S. Arulananda Babu) Post-doc with Prof. Lei Wang (University of California, SF) at Hangzhou branch of Technical Institute of Physics and Chemistry, Chinese Academy of Sciences.

Alumni Placements

Dr. Vadla Rajkumar	2016	(Dr. S. Arulananda Babu), at GVK BioSciences, Hyderabad.
Dr. Chennakesava Reddy	2016	(Dr. S. Arulananda Babu) Post-doc, IISER, Pune.
Dr. Kuldeep Jaiswal	2016	(Dr. Sanjay Singh) working at Nankai University, China as a Post-doc fellow.
Dr. B. T. Ramanjaneyulu	2016	(Dr. R. Vijaya Anand), Senior Scientist, DongSung Bio Pharmaceutical Co., Ltd., South Korea.
Dr. Sumyra Sidiq	2016	(Dr. S. K. Pal) Assistant Professor, Government degree college for women, University of Kashmir.
Dr. Shilpa Setia	2016	(Dr. S. K. Pal) Bhag Singh Khalsa College for Women, Abohor, Punjab.
Dr. Naveen	2017	(Dr. S. Arulananda Babu) Post-doc, Weizmann Institute of Science, Israel.
Dr. R. Parella	2017	(Dr. S. Arulananda Babu) Post-doc, University of Texas, USA.
Dr. B. Gopalakrishnan	2017	(Dr. S. Arulananda Babu) Post-doc, IIT Madras, India.
Dr. V. Venkat Reddy	2017	(Dr. R. Vijaya Anand), Senior Research Investigator (Team Leader), Syngene International Ltd., Hyderabad.
Dr. Panjab B. Arde	2017	(Dr. R. Vijaya Anand), N.A.
Dr. Mahesh Sriram	2017	(Dr. R. Vijaya Anand) Post-doc fellow at the University of Auburn, USA.
Dr. Hare Ram Yadav	2017	(Dr. Angshuman Roy Choudhury) Working at SNU as X-ray facility manager.
Dr. Shruti Arya	2017	(Dr. Samrat Mukhopadhyay), Post-doc, Univ. of California, Santa Barbara.
Dr. Monika Gupta	2018	(Dr. S. K. Pal) Post-doc fellow in the University of Tokyo, Japan.
Dr. Abhijeet S. Jadhav	2018	(Dr. R. Vijaya Anand) Research Scientist at Sphaera Pharma Pvt. Ltd., Gurugram, Haryana.
Dr. Prithwish Goswami	2018	(Dr. R. Vijaya Anand) Post-doc at UNIST, South Korea.
Dr. Moumita Rana	2018	(Dr. Ujjal K. Gautam) Post-doc., IMDEA Materials Institute, Madrid.
Dr. Sudha Devi	2018	(Dr. Sugumar V) College Lecturer.
Dr. Deependra Bawari	2018	(Dr. Sanjay Singh) Post-doc fellow at UMR-CNRS at Tolouse, France.
Dr. Karishma Bhasne	2018	(Dr. Samrat Mukhopadhyay), Post-doc at University of Massachusetts, USA.
Dr. R. Sankar	2018	((Dr. S. Arulananda Babu) Associate Scientist at 'GVK BIO' Pharma and also received the Kothari Post-doc Fellowship.
Dr. Ginny Karir	2018	(Prof. K. S. Viswanathan), Post-doc at Ruhr University, Bochum, Germany.
Dr. Kanupriya Verma	2018	(Prof. K. S. Viswanathan), Post-doc at Purdue University, USA (2018-2019).
Dr. Narendra Bisht	2019	(Dr. S. Arulananda Babu) Scientist at Jubilant Chemsys Ltd, Noida.
Dr. Sandeep Kumar	2019	(Prof. Sanjay Mandal), Post-doc: Harbin Institute of Technology, China.
Dr. Vijay Gupta	2019	(Prof. Sanjay Mandal), Post-doc: University, Polish Academy of Sciences, Warsaw (PAN), Poland.
Dr. Prasenjit Das	2019	(Prof. Sanjay Mandal), Post-doc: University of Pittsburgh, USA.
Dr. Gouri Chakraborti	2019	(Prof. Sanjay Mandal), Post-doc: University, Singapore.
Dr. Datta Markad	2019	(Prof. Sanjay Mandal), Post-doc: University of Liverpool, UK.
Dr. Smriti Thakur	2019	(Prof. Sanjay Mandal), Post-doc: IIT Mandi.
Dr. Jyoti Saini	2019	(Prof. K. S. Viswanathan) Faculty,Sardar Vallabhbhai National Institute of Technology, Surat, Gujarat.
Dr. Pankaj Dubey	2019	(Prof. K. S. Viswanathan) Post-doc, Indian Institute of Technology, Gandhinagar, Gujarat.
Dr. Vinay Ganapathy	2019	(Dr. R. Ramachandran), Post-doc at TCIS, Hyderabad.
Dr. Bishnupada Satpathi	2019	(Dr. S. S. V. Ramasastry) Post-doc, University of North Carolina.
Dr. Siddheswar K. Bankar	2019	(Dr. S. S. V. Ramasastry) Post-doc, University of Utah (to be joining).
Dr. Rajendra Shirke	2019	(Dr. S. S. V. Ramasastry) Post-doc, Seoul University (to be joining).

Awards/Honours/Achievements/Recognitions

Faculty

- Jino George has received the MHRD-STARS grant 2020.
- S Maiti and Santanu K Pal have received the MHRD-STARS grant 2020.
- DST-FIST Application (2019) was defended (by S A Babu (Head, DCS), S. Singh and A K De) and the Department has received the sanction for Departmental NMR Research facility.
- Samrat Mukhopadhyay was appointed in the Editorial Board Members of Biophysical Journal in the year 2020. Samrat Mukhopadhyay has been appointed to the Editorial Advisory Board of the Journal of Physical Chemistry, American Chemical Society (2019-2021).
- Santanu K Pal has received the Chemical Research Society of India (CRSI) Bronze Medal for the year 2020.
- DST/Early Career Award (2019) was received by S Maiti and Raj Kumar Roy.
- Monika Sharma has received Bharat Vikas Award for the year 2019.
- Samrat Mukhopadhyay has received the Chemical Research Society of India (CRSI) Bronze Medal for the year 2019.
- DST/Early Career Award (2017) was received by Debashis A.
- Rama Sastry Sripada has received the DST-Swarnajayanti Fellowship for the year 2018. Rama Sastry Sripada has received the Chemical Research Society of India (CRSI) Bronze Medal for the year 2018. Rama Sastry Sripada has received Thieme Chemistry Journal's Award 2017 [Chosen by the Editorial Boards of Synlett, Synthesis and Synfacts] (2017).
- Arijit Kumar De has received DST travel fellowship to attend Gordon Conference on "Quantum Control of Light and Matter", USA. (Application No. - ITS/Off-502/2017-18) (2017).
- Arijit Kumar De has received INSA travel fellowship to attend Gordon Conference on "Quantum Control of Light and Matter", USA. (INSA travel Grant No. SS/INSA/2017/758) (2017).
- Balanarayan P. received the best teacher's award from IISER Mohali (2017).
- Arijit Kumar De has received SERB, DST Early Career Research Award. (Grant No: ECR/2016/000467) (2016).
- S. V. Rama Sastry Sripada has received the young scientist award from the organizing committee of "Chemical Frontiers" (2016).
- S. V. Rama Sastry Sripada has been admitted as a Member of the Royal Society of Chemistry (MRSC) (2016).
- Sabyasachi Rakshit has received Wellcome Trust/DBT Intermediate Fellowship, DBT. (2015).
- 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 Ramachandran 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/Honours/Achievements/Recognitions

Students & Postdocs/RA's

Ms. Anjana R. Kamath (5th Year BSMS student) received the DAAD Fellowship-2019.

Ms. Labhini received the Best Poster Award in the'16th conference of the Asian Crystallographic Association', held in Singapore (2019).

Dr. Gayathri S Singaraju received International Travel Award by EMBO (European Molecular Biology Organisation.

Mr. Jagadish P Hazra received International Travel Award and Invitation for an Oral presentation in the Biophysical Society Meeting, 2019, USA.

Ms. Samita Mishra received ACS Omega Award, 26th CRSI National Symposium in Chemistry, 2020.

Ms. Sakshi Chawla received ACS Applied Energy Materials Award, 26th CRSI National Symposium in Chemistry, 2020.

Mr. Jaibir S received the SPM PhD fellowship from CSIR.

Mr. Mayank Saraswat: Selected for the forthcoming 70th Nobel Laureates meeting at Lindau, Germany through DST.

Dr. Subhash Chander (post-doc): ACS CAS Future Leaders Program Award, 2019. Link from ACS.

Ms. Yogita Silori has received the International Travel Support (ITS) from Science and Engineering Research Board, DST for attending photochemistry Gordon Research Conference at Stonehill College, Massachusetts, USA (2019).

Ms. Anita Devi has received the travel grant from International Travel Support (ITS) from Science and Engineering Research Board, DST for CLEO/Euorope-EQEC at Munich, Germany (2019).

Ms. Priyanka Dogra, a PhD student in the lab, has received the international travel award from the European Molecular Biology Organization (EMBO) to attend the EMBO phase separation workshop that will be held at Max Planck Institute, Dresden, Germany in February 2019.

Dr. Anupa Majumdar, a National Postdoc Fellow has been selected for an oral presentation at the Biophysical Society meeting that will be held in Baltimore, USA in February 2019.

Mr. Jagadish P Hazra received the Best Poster Award during ACS on Campus, Feb 2018. Mr. Jagadish P Hazra received the Best Poster Award in FCS 2018, Nov 2018. Mr. Jagadish P Hazra received BPS Travel Grant, USA, 2018.

Ms. Shaina Dhamija has received travel grant from "Society de Biophysique" (Biophysical Society of Canada) for attending Faraday Discussions (on Photoinduced Processes in Nucleic Acids and Proteins) at Trivandrum, India (2018).

Ms. Harleen Kaur received the best poster award in "Chemistry Conference for Young Scientists" held in Blankenberge, Belgium (2018).

Mr. Bishnu S received the best oral presentation award and Mr. Rajendra S received the best poster presentation award during the 'Emerging Trends in Drugs Development and Natural Products (ETDDNP 2018)' conference held at the University of Delhi during 12-14 Jan, 2018.

Ms. Ipsita Pani received the best poster award at "ACS in Campus" Roadshow in February, 2018 held at IISER Mohali.

Ms. Indu Bala and Ms. Ipsita Pani received the registration fee and travel support to attend the workshop titled "Soft and Active Matter" scheduled from 11th – 17th February 2018 organized at UGC-Networking Resource Centre (UGC-NRC), School of Physics, University of Hyderabad, Hyderabad.

Ms. Indu Verma's liquid crystal picture was selected as the featured artwork of June 2018 in International Liquid Crystal Society (ILCS) website.

Ms. Nazma Begum's liquid crystal picture has been selected as the featured artwork of December 2018 in International Liquid Crystal Society (ILCS) website.

Mr. Joydip De was awarded International Travel Support from Department of Science and Technology (DST) for attending International Liquid Crystal Conference (ILCC) 2018, held at Kyoto, Japan.

Ms. Indu Verma, Ms. Indu Bala and Mr. Joydip De were awarded International Liquid Crystal Conference (ILCC) 2018 registration fee waiver by Liquid Crystal Institute (LCI), Kent State University (KSU), USA for attending International Liquid Crystal Conference (ILCC) 2018 held at Kyoto, Japan.

Dr. Rajib Kumar Nandi, received Best Poster Award in National Post Doctoral Fellow (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 National Institute of Plant Genome Research (NIPGR), New Delhi on July 25, 2018.

Awards/Honours/Achievements/Recognitions

Ms. Vidhika Punjani received the ACS best poster award at “Frontiers in Chemical Sciences (FICS) 2018” in December 2018 held at IIT Guwahati.

Ankit Somani (BS-MS student) received best poster @IINCM2017, Dec 2017 held at NISER Bhubaneswar,

Mr. Deependra Bawari (PhD student) has been awarded an "MTIC" best poster award at the 17th symposium of 'Modern Trends in Inorganic Chemistry (MTIC-VII)' held at CSIR-NCL, Pune and IISER Pune during 11-14 December, 2017.

Mr. Bishnupada Sathpathi received the BEST poster award from the organisers of the 'Thematic Conference in Chemical Sciences (TC2S-2017): Sustainable Chemistry' held at IIT Ropar during May 15-16, 2017.

Mr. Deependra Bawari 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). (2017)

Mr. Deependra Bawari attended the 11th International Symposium on Macrocyclic and Supramolecular Chemistry, 10-14 July, 2016. Travel support by IISER Mohali. (2016)

Ms. Seema Dhiman received the Eli-Lilly Outstanding Thesis Award-2016.

Dr. Anamika Mukhopadhyay (Postdoc) has received CSIR Pool Scientist award. (2015)

Ms. Indu Verma 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)

Ms. Sumyra Sidiq has received International Travel award from DST-SERB to attend International Liquid crystal conference (ILCC) held in Trinity college, Dublin, Ireland. (2014)

Ms. Gurpreet Kaur has received best oral presentation award in 42nd National Seminar on Crystallography held in JNU, New Delhi. (2013)

Ms. Sadhika Khullar 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).

Ms. Shilpa Setia won The Dewan Jawahar Lal Nayar Memorial prize at the 20th National Conference on Liquid Crystals (NCLC) (best poster presentation). (2013)

Ms. Sumyra Sidiq 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)

Ms. Gurpreet Kaur has received Best poster award in 20th International Conference on the Chemistry of Organic Solid State held in IISc Bangalore. (2010)

Awards/Honours/Achievements/Recognitions

Sudents & Postdocs/RA's

The following BS-MS students received fellowsips 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) VSRP fellowship
16	Anjana/MS15	CUSAT, Cochin	2016	Summer Internship
17	Priyanka Bansal/MS13	Indiana University, USA	2017	Summer Internship
18	Divita Gupta/MS13	University of Rennes 1, France	2017	VSRP fellowship
19	Rishabh Gupta/MS14	TIFR Hyderabad	2017	
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	IITBombay	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

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 roots of this club go back about four years, when some of the students of the Chemistry Majors decided to meet every Saturday to discuss recent advancements in Chemistry. The club was christened as 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.

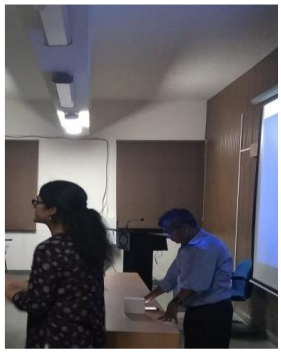
The club has active participation from undergraduates, graduates and faculty. The activities organized by the club are scientific talks, both by speakers within IISER and other institutions. Students are encouraged to talk about their project work, demonstrate novel experiments and disseminate their knowledge during outreach programmes, such as the KVPY camp and National Science Day. Curie club also screens Nobel lectures and documentaries, which are followed by discussions. Curie Club has also been organizing industrial visits to provide an exposure to students for the applications of Chemistry in the industry.

Every year, sometime in September, the club organizes the 'Guess the Laureate' contest, inviting participants to predict the Chemistry Nobel Prize winner of that year. This contest aims at increasing the awareness regarding the ground breaking research, in different fields of chemistry. The contest is open to all the IISERs, NISER, INST, IICT and IISc among other institutions.

Curie Club also celebrates a week long event called the 'Chem Week' during the first week of November every year, to commemorate the birth anniversary of Sir CV Raman and Madam Marie Curie, both of which fall on the Nov 7. The events during the week include talks and interactive sessions by eminent scientists, activities such as descriptive writing, quiz, 'just a minute' (JAM), game of taboo, poster presentation, model making and sketching.

The club has been recording the videos of all the events that have been organized and these are available online on Curie Club's YouTube channel (Curie Club IISER Mohali). The club intends to reach a large section of the scientific community through these videos and also encourage students in the pursuit of science.

Curie Club Activities



The People

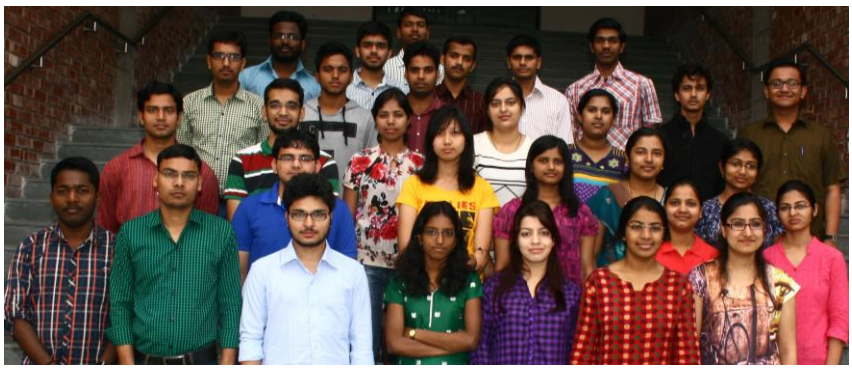
MS08 batch Students

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

Teaching lab and DCS Office Assistants:

Lab assistants/attendants: (L to R) Mr. Mangat Ram, Mr. Khem Bahadur, Mr. Ajay Sharma, Mr. Chetan Kumar Gaur, Mr. Prahlad Singh, Mr. Satwinder, and Mr. Triveni Shanker (top right) DCS Office assistant: Mr. Rahul Saini (bottom right)

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