Department of

# CHEMICAL SCIENCES

# 2017

**Indian Institute of Science Education and Research Mohali**

# Messages from the Director's and Head's Desk

I am delighted to see that the Department of Chemical Sciences at IISER Mohali is bringing out its Faculty Profile. It was a considered decision of the Institute to form a few generic departments, for the purpose of teaching administration. Therefore, it is not surprising that some of the colleagues in chemical sciences could have been in the department of physical sciences or biological sciences. The composition of the department cuts across subdisciplines, reflecting the changing times. The faculty tries to understand the principles of chemical structure and dynamics and use them in creating new materials that would have valuable properties. While pursuing knowledge is the stated motto of the institute, transforming knowledge into wealth is the order of the day. Understandably, most of the patents filed by the institute come from one department, that of chemical sciences. I wish the young vibrant faculty and the students of the department all the best in their endeavour.

N. Sathyamurthy
Professor & Director,
IISER Mohali

It is with enormous delight and pride that we present this brochure of the Department of Chemical Sciences, IISER, Mohali. This Department embodies everything that one expects to see in an academic set up – faculty committed to their research and teaching, and an enthusiastic group of students. As this brochure will highlight, the research conducted in the Department is in very diverse areas, which can only get more varied in the years to come. In teaching, we place a strong emphasis on both class room lectures and laboratory work, where our students receive hands-on experience on many of the sophisticated experimental techniques. Consequently they are well prepared for a scientific career in academia and industry. No less an importance is placed on ethics in the education process. We have no doubt that our students will do us proud in the years to come and our faculty will reach great heights. This Department is a happy family of faculty and students that aims at furthering the horizons of science.

K. S. Viswanathan
Professor & Head

# Table of contents

**N. Sathyamurthy, FNA, FASc, FTWAS**
**Professor & Director**
E-mail: nsath@iisermohali.ac.in
Tel: +91 9779144905

# Theoretical/Computational Chemistry

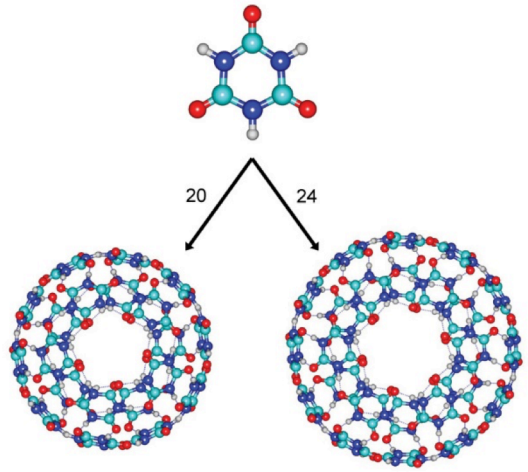
**Profile:**

**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.

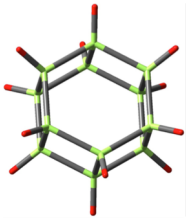
More recently, Sathyamurthy and his students have been investigating the structure and stability of water clusters, boric acid clusters, endohedral fullerenes, and gas hydrates. The role of structural motifs in deciding the shapes of clusters has been the focus of attention. The results on gas hydrates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

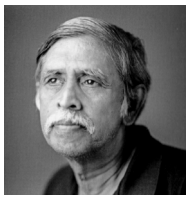
(2) Stabilisation of the [6]-prismane structure by silicon substitution, A. Equbal, S. Srinivasan and N. Sathyamurthy, *J. Chem. Sci.* (Special issue in honor of Charusita Chakravarty) **2017**, 129, 911-917.

(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.

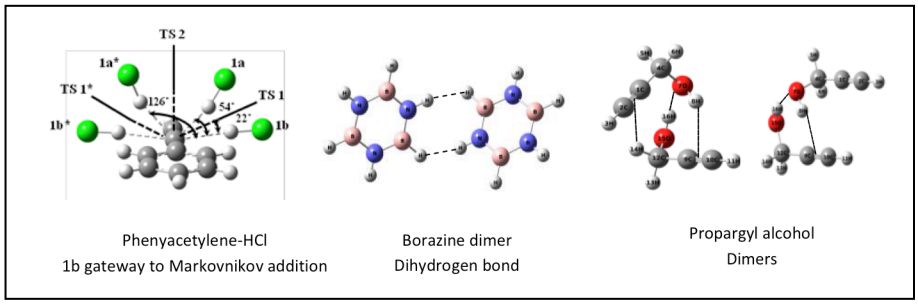
**K. S. Viswanathan**
**Professor & Head**
E-mail: vish@iisermohali.ac.in
Tel: +91 9530802088



# Matrix Isolation Infrared Spectroscopy

**Profile:**

**Ph.D** – 1983/Vanderbilt University,USA.
Supervisor: Prof. Joel Tellinghuisen
**Postdoc**–1983-85/Indiana Univ. USA
Supervisor: 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), Ms. Ginny, Ms. Kanupriya, Ms. Jyoti, Mr. Pankaj (PhD researchers), Mr. Mrinal, Mr. Gaurav, Dr. Kapil, Mr. Deepak, Ms. Mariyam, Mr. Piyush, Mr. Akshay, Ms. Gargi, Mr. Srijit, Ms. Shruti, Mr. Ravi, Mr. Sumit, Ms. Priyanka, Ms. Divita, Ms. Amala (Masters researchers).

**Non-Covalent Interactions:** Study of hydrogen bonded interactions is an important area of research we do. We particularly 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, not observed earlier, (except in systems involving a metal hydride).

Study of propargyl alcohol and propargyl amine systems highlighted the interplay of interactions in complexes with multiple contacts. Propargyl alcohol dimers were also studied which identified two isomers, a study 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 and systems of relevance to astrochemistry.

**Selected Publications**

**(1)** "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

**(2)** "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

**(3)** Study of the Propargyl Alcohol Dimers, Jyoti Saini, K. S. Viswanathan, *J. Phys. Chem. A* **2017,** *121*, 1448

**(4)** "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, DOI:** 10.1080/00268976.2017.1284357

**(5)** "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

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

**(7)** Matrix Isolation Spectroscopy-A Window to Molecular Process. Pankaj Dubey, Jyoti Saini, Kanupriya Verma, Ginny Karir, Anamika Mukhopadhyay, K. S. Viswanathan, Molecular and Laser Spectroscopy. **2017**, **DOI**:10.1016/B978-0-12-849883-5.00014-0 (Book Chapter)

**(8)** Conformations of L-Threonine" Pankaj Dubey, Anamika Mukhopadhyay, K. S. Viswanathan, (manuscript in preparation)

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

**Sanjay K. Mandal**
**Professor**
E-mail: sanjaymandal@iisermohali.ac.in
Tel: +91 172-2293198 (office); 172-2293185 (lab)

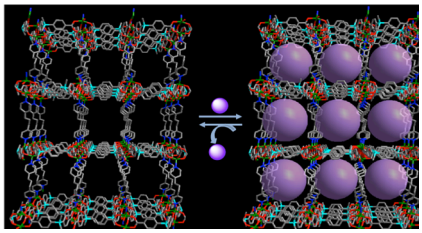
# Inorganic/Organometallic Chemistry and X-ray Crystallography

**Profile:**

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

**Research Interests:**

Prof. Mandal's group is engaged in developing diversified chemistry of elements across the periodic table through a variety of interdisciplinary projects that involve multi-step organic synthesis, coordination chemistry, catalysis and materials chemistry. Various spectroscopic techniques (UV-vis, FTIR, NMR, Raman, CD and Fluorescence), thermal analysis (TGA and DSC), electrochemistry and X-ray crystallography (PXRD and SCXRD) are routinely used for establishing physicochemical properties of the new organic, inorganic and organometallic compounds. This has resulted in the strategic design of coordination architectures with a special emphasis on Metal Organic Frameworks (MOFs) for their diverse structural aesthetics and for their possible roles in various applications, such as catalysis, molecular 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 of carbon dioxide (lowering greenhouse effect), (iv) chormogenic and/or fluorogenic sensing of the cations, anions and neutral small molecules at the ppm or ppb level, (v) chiral catalysis, and (vi) generation and applications of metal oxides, sulfides and selenides in luminescence, photocatalysis and quantum dots.



Schematic drawing of Host-Guest chemistry in porous MOFs.

**Selected Publications:**

**(1)** "Construction of a Robust Pillared-layer Framework Based on the Rare Paddlewheel Subunit $[Mn^{II}_2(\mu\text{-}O_2CR)_4L_2]$: Synthesis, Crystal Structure and Magnetic Properties", V. Gupta, S. Khullar, S. Kumar, and S. K. Mandal, *Dalton Trans.,* **2015**, c5dt02354h.

**(2)** "Controlling the Self-assembly of Homochiral Coordination Architectures of $Cu^{II}$ by the Substitution in Amino Acid Based Ligands: Synthesis, Crystal Structures and Physicochemical Properties", N. Kumar, S. Khullar and S. K. Mandal, *Dalton Trans.,* **2015**, 5672.

**(3)** "Solvent Effect on Neutral Chiral Supramolecular Assemblies and Their Distinct Receptor Behaviour Towards Anions", N. Kumar, S. Khullar and S. K. Mandal, *Dalton Trans.,* **2015**, 1520.

**(4)** "Ancillary Ligand Assisted Self-assembly of Coordination Architectures of Mn(II): the Effect of the *N*-alkyl Group on a Tridentate Ligand", S. Khullar and S. K. Mandal, *Dalton Trans.,* **2014,** *44*, 1203.

**(5)** "Structural Diversity of the Encapsulated Water Clusters in the 3D Supramolecular Assemblies: a Cyclic Quasi-planar Hexamer of Water Constructed Through Strong Hydrogen Bonding Interactions", S. Khullar and S. K. Mandal**,** *CrystEnggComm*, **2013**, *15*, 6652.

**(6)** "Supramolecular Assemblies of Dimanganese Subunits and Water Clusters Organized by Strong Hydrogen Bonding Interactions: Single Crystal to Single Crystal Transformation by Thermal De/Rehydration Processes", S. Khullar and S. K. Mandal, *Cryst. Growth Des*., **2012**, *12*, 5329.

**(7)** "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.

From left: Sandeep, Sandhya, Shradha, Gouri, Alisha, Smriti, Prasenjit, Datta, Biswajit, Sanjay, Vijay, Sheeba

**Samrat Mukhopadhyay**
**Associate Professor**
E-mail: mukhopadhyay@iisermohali.ac.in
Tel: +91-172-2293150

# Molecular Biophysics

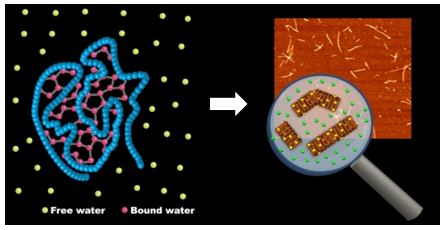
**Profile:**

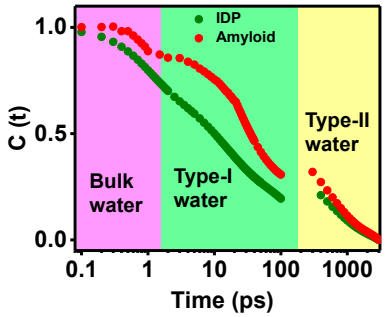
**Ph.D.** – 2000-2004/Indian Institute of Science, Bangalore
**Visiting Fellow** – 2004-05/Tata Institute of Fundamental Research, Mumbai
**Postdoc** – 2005-2008/The Scripps Research Institute, La Jolla, California, USA
**Professional experience** – 2008-13/Assistant Professor, IISER Mohali
2013-present/Associate 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:**

Intrinsically disordered proteins (IDPs) belong to the emerging class of proteins that do not undergo autonomous folding into a well-defined 3D structure and challenge the tenets of traditional sequence-structure-function paradigm. They are associated with a number of important cellular functions and devastating human diseases. The Mukhopadhyay laboratory at IISER Mohali is involved in addressing some important and intriguing structural, dynamical, nanoscopic and mechanistic issues of prion and amyloid-forming IDPs. Amyloid formation is linked with a variety of debilitating human disorders such as Alzheimer's, Parkinson's and prion diseases. The transition from a normal functional protein to an altered (misfolded) form often involves a profound conformational change that triggers the aberrant protein assembly resulting in a wide variety of nanostructures including amyloid oligomers, pores and fibrils. The laboratory utilizes a diverse array of methodologies to unravel the key molecular events that are crucial in amyloid formation from a number of disease-associated proteins.

Recently, using femtosecond and picosecond time-resolved fluorescence spectroscopy, in conjunction with all-atom molecular dynamics simulations, we have embarked upon collaborative studies aimed at unraveling the crucial role of hydration water in amyloid formation.




"Water Rearrangements upon Disorder-to-Order Amyloid Transition" S. Arya, A. K. Singh, T. Khan, M. Bhattacharya, A. Datta, & S. Mukhopadhyay *J. Phys. Chem. Lett.* **2016**, *7*, 4105-4110.

**Selected Publications:**

**(1)** "pH-Responsive Mechanistic Switch Regulates the Formation of Dendritic and Fibrillar Nanostructures of a Functional Amyloid" P. Dogra, M. Bhattacharya & S. Mukhopadhyay *J. Phys. Chem. B.* **2017**, *121*, 412–419.
**(2)** "Water Rearrangements upon Disorder-to-Order Amyloid Transition" S. Arya, A. K. Singh, T. Khan, M. Bhattacharya, A. Datta, & S. Mukhopadhyay *J. Phys. Chem. Lett.* **2016**, *7*, 4105-4110.
**(3)** "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.
**(4)** "Confined Water in Amyloid-Competent Oligomers of the Prion Protein" V. Dalal, S. Arya, & S. Mukhopadhyay *ChemPhysChem* **2016**, *17*, 2804-2807.
**(5)** "Conformational Switching and Nanoscale Assembly of Human Prion Protein into Polymorphic Amyloids via Structurally-Labile Oligomers" V. Dalal, S. Arya, M. Bhattacharya & S. Mukhopadhyay *Biochemistry* **2015**, *54*, 7505–7513.

**Sanjay Singh**
**Associate Professor**
E-mail: sanjaysingh@iisermohali.ac.in
Tel: +91 9878470451

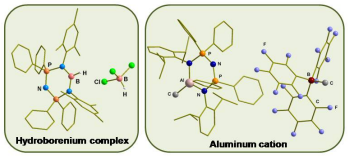
# Organometallic & Macrocyclic Chemistry

**Profile:**

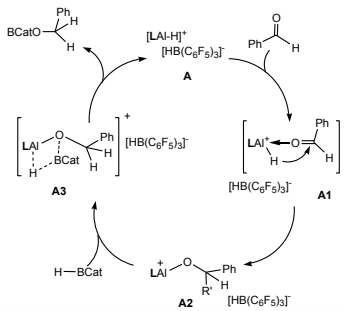
**PhD** – 2003-06/University of Göttingen Göttingen, Germany /Prof. H. W. Roesky
**Postdoc**–January-November 2006/University of Göttingen, Göttingen, Germany /Prof. H. W. Roesky
**Postdoc**–December 2006-November 2007/University of Cambridge, Cambridge, England /Prof. D. S. Wright
**Professional experience**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

**Research Interests:**

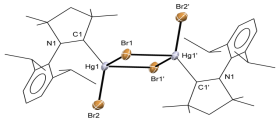
**(1) Chemistry of group 13 elements: Hydridoborenium complexes and their aluminum congeners for main group catalysis**




Synthesis of highly reactive three coordinated cationic hydridoborane and aluminum hydrides or alkyls, supported by bulky ligands with $N_2P$ or $N_3P_2$ skeleton, is major emphasis of this research. A series of hydridoborenium ions and aluminum congeners with weakly coordinating anions have been isolated. Applications of these cations in Lewis acid mediated hydroboration (shown below with AlH cation) and hydrosilylation have been successfully explored.

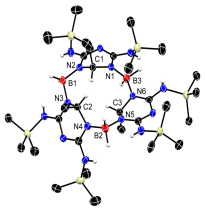



**(2) cAAC and *N*-heterocyclic carbene complexes of transition elements for catalysis:** cAAC and NHC carbene complexes of late transition elements (Pd, Au, Zn, Hg etc.) have been investigated in this project. The high activity of cAAC-$HgBr_2$ adduct in the intermolecular hydroamination of alkynes and good activity of a Pd(II) complex in mono- and bis-arylation of methylacrylate with arylbromides in Heck type coupling are noteworthy.



**(3) Inorganic macrocycles 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 and 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; 2016-2018
Amount: Rs. 52,43,575.

**Selected Publications:**

**(1)** "Product Isomer Distribution in the Sequential Functionalization of Cyclic-$(P^{III})_2N_2$ Framework" D. Bawari, B. Prashanth, K. Jaiswal, A. R. Choudhury, S. Singh*, *Eur. J. Inorg. Chem*. **2017**, 10.1002/ejic.201700855.

**(2)** "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.

**(3)** "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*.

**(4)** "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.

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

**(6)** "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: Mamta, Chandrakala, Pragati and Deepika.*

*second row: Soumyadeep, Sandeep Rawat and Sandeep Thakur*

*third row: Vishal, Deependra, Sanjay and Nitish*

**Ramesh Ramachandran**
**Associate Professor**
E-mail: rramesh@iisermohali.ac.in
Tel: +91 9878552865

# 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

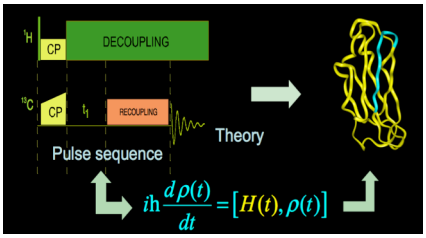
(b) Time dependent Quantum mechanics

(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**
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.

**Research Interests:**

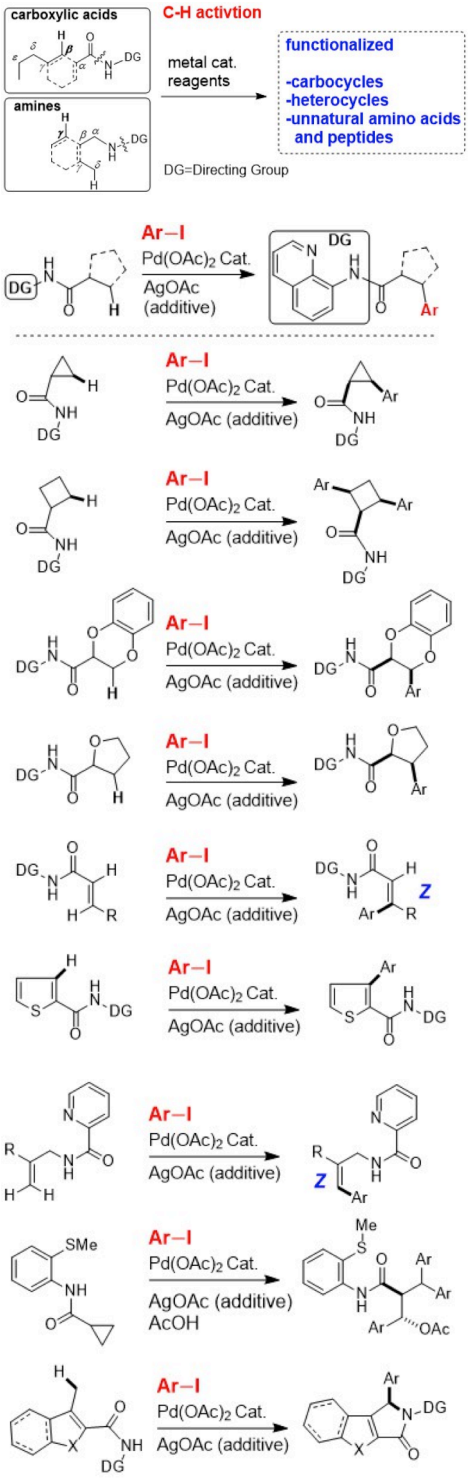
C-H Activation Reactions.

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 (Ongoing, 2015-2018)




**Selected Publications:**

(1) "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.

(2) "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.

(3) "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.

(4) "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.

(5) "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.

(6) "Direct Bis-Arylation of Cyclobutanecarboxamide via Double C–H Activation: An Auxiliary-Aided Diastereoselective Pd-Catalyzed Access to Trisubstituted Cyclobutane Scaffolds Having Three Contiguous Stereocenters and an All-cis Stereochemistry" Parella, R., Gopalakrishnan, B., Babu, S. A., *J. Org. Chem.*, **2013**, *78*, 11911.

**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

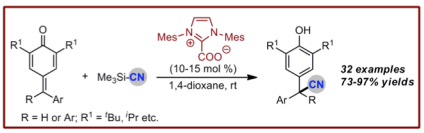
## Profile:

**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)

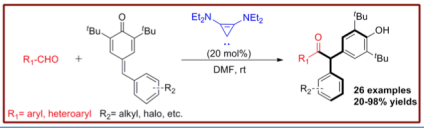
## Research Interests:

### 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. An interesting approach has been described for the synthesis of α-arylated nitriles through 1,6-conjugate addition of TMSCN to *p*-quinone methides (*p*-QMs) and fuchsones using NHC as a catalyst.

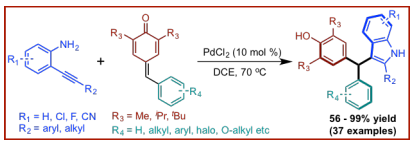



Another interesting methodology, which involves synthesis of α,α'-diarylated ketones through BAC catalyzed 1,6-conjugate addition of aldehydes to *p*-QMs, has been developed in our lab.



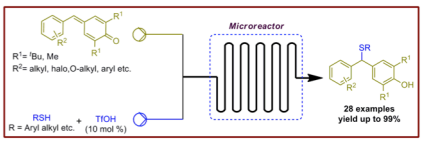

### 2) Metal-catalyzed Domino Cyclization reactions

we have recently developed an efficient method for the synthesis of unsymmetrical diarylindolylmethanes through Pd-catalyzed cyclization of 2-alkynyl anilines followed by trapping with *p*-QMs.




### 3) Continuous-flow reactions

An interesting methodology has been developed under continuous flow conditions to access diarylmethyl thioethers through a triflic acid catalyzed vinylogous Michael addition of aromatic and aliphatic thiols to *p*-quinone methides.




***External Funding (ongoing):***
Funding Agency: DST – SERB
Duration: 2016-19
Amount: Rs. 49.5 Lakhs

*Back row (from left): Yogesh, Pavit, Abhijeet, Prithwish and Feroz.*

*Front row (from left): Sonam, Rekha, Swati, Dilip, Mahesh and Vijay.*

## Selected Publications:

**(1)** "N-Heterocyclic carbene catalyzed 1,6-conjugate addition of $Me_3Si$-CN to *para*-quinone methides and fuchsones: Access to α-arylated nitriles" Goswami, P.; Singh, G; Anand, R. V.* *Org. Lett*. **2017**, *19*, 1982.
**(2)** "TfOH catalyzed 1,6-conjugate addition of thiols to *p*-quinone methides under continuous-flow conditions" Jadhav, A. S.; Anand, R. V.* *Eur. J. Org. Chem*. **2017**, 3716.
(Invited article: Emerging investigators from India in summer 2017]
**(3)** "1,6-Conjugate addition of Zinc alkyls to *para*-quinone methides in a continuous-flow microreactor" Jadhav, A. S.; Anand, R. V.* *Org. Biomol. Chem*. **2017**, *15*, 56.
**(4)** "Cu-catalyzed hydrophosphonylation of 2-(2-enynyl)pyridines: Easy access to indolizine containing diarylmethyl-phosphonates" Mahesh, S.; Anand, R. V.* *Eur. J. Org. Chem*. **2017**, 2698.
**(5)** "*N*-Heterocyclic carbene catalysed 1,6-hydrophosphonylation of *p*-quinone methides and fuchsones: An atom economical route to unsymmetrical diaryl- and triarylmethyl phosphonates" Arde, P; Anand, R. V.* *Org. Biomol. Chem*. **2016**, *14*, 5550.
(Invited article: New Talent)
**(6)** "Bis-(amino)cyclopropenylidene-catalyzed 1,6-conjugate addition of aromatic aldehydes to *p*-quinone methides: Expedient access to α,α'-diarylated ketones" Ramanjaneyulu, B. T.; Mahesh, S.; Anand, R. V.* *Org. Lett*. **2015**, 17, 3952.
**(7)** "An expedient access to unsymmetrical diaryindolylmethanes through palladium catalyzed domino electrophilic cyclization - extended conjugate addition approach" Reddy, V.; Anand, R. V.* *Org. Lett*. **2015**, *17*, 3390.
**(8)** "*N*-Heterocyclic carbene catalyzed highly chemoselective intermolecular crossed acyloin condensation of aromatic aldehydes with trifluoro-acetaldehyde ethyl hemiacetal" Ramanjaneyulu, B. T.; Mahesh, S.; Anand, R. V.* *Org. Lett*. **2015**, *17*, 6.

**Santanu Kumar Pal**
**Associate Professor**
E-mail: skpal@iisermohali.ac.in
Tel: +919501047835

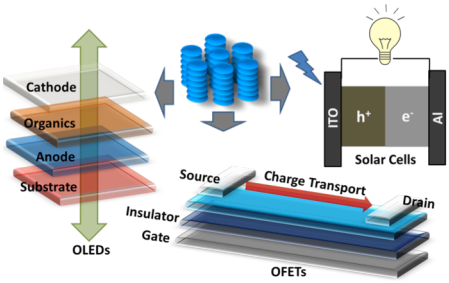
# Supramolecular Chemistry

**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:**

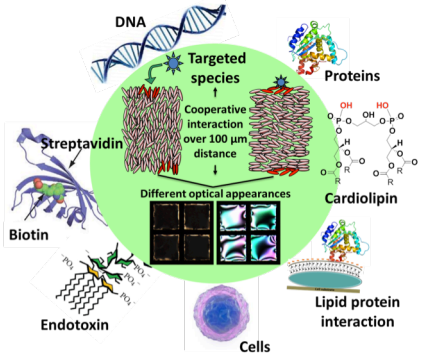
**Liquid Crystal nanocrystals: Functional materials for electronic devices:**




Electronic devices based on organic semiconductors have gained increased attention in the field of FETs 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 sought to design new room temperature 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.

**Nano-channels for efficient Proton Conduction:**

In this project our aim is to synthesize new LCs and covalent organic frameworks having a balance between required supra-molecular organization of proton-conducting groups and flexibility for molecular reorientation. These systems will provide a viable platform for developing efficient proton transporting materials.

Funding: CSIR, INSA, DAE-BRNS, IISER Mohali

**Selected Publications:**

**(1)** "A new strategy towards the synthesis of a room-temperature discotic nematic liquid crystal 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.

**(2)** "Poly(L-lysine)-Coated Liquid Crystal Droplets for Cell-Based Sensing Applications" S. Sidiq, G. V. R. Krishna Prasad, A. Mukhopadhaya, **S. K. Pal*** *J. Phys. Chem. B*, **2017**, *121*, 4247.

**(3)** "Room-temperature oligomeric discotic nematic liquid crystals over a wide temperature range: Structure-property relationships" M. Gupta, S. P. Gupta, S. S. Mohapatra, S. Dhara, **S. K. Pal*** *Chem. Eur. J.*, **2017,** DOI: 10.1002/chem.201701578

**(4)** "Room temperature columnar nematic and soft crystalline columnar assemblies of a new series of perylene-centered disc tetramers" I. Bala, S. P. Gupta, J. De, **S. K Pal*** *Chem. Eur. J.*, **2017,** DOI: 10.1002/chem.201702181

**(5)** "TNF Induced Switching of Columnar Rectangular to Hexagonal Assemblies in a New Class of Triphenylene-Based Room Temperature Discotic Liquid Crystals" M. Gupta, S. P. Gupta, **S. K. Pal*** *J. Phys. Chem. B,* ***2017.*** DOI:10.1021/acs.jpcb.7b06737.

**(6)** "Triphenylene-Based Room-Temperature Discotic Liquid Crystals: A New Class of Blue-Light-Emitting Materials with Long-Range Columnar Self Assembly Gupta, M ; **Pal, S. K.*** *Langmuir,* **2016**, 32, 1120.

Group members: Golam, Harpreet, Santanu, Neelima, Swathy, Joydip, Rajib, Monika, Indu Verma, Indu Bala, Nitya, Supreet, Lisha, Vaishnavi, Musthafa, Vidhika, dibyendu, Varsha, Ipsita.

**Sripada S. V. Rama Sastry**
**Associate Professor**
E-mail: ramsastry@iisermohali.ac.in
Tel: +91 96461-73747

# 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:**

**i)** Development of stereoselective reactions with relevance to both medicinal and natural products chemistry with particular emphasis on

- BrØnsted and Lewis acid catalysis.
- Asymmetric organocatalysis

**ii)** Development of green and sustainable synthetic chemistry, and atom economic reactions.

**iii)** Application of aforementioned strategies in the total synthesis of bioactive natural products and pharmaceutically important compounds.

**iv)** Collaborative efforts for the development of medicinal chemistry aspects and chemoinformatics.

***Currently ongoing projects***

- Development of multicatalytic and multicomponent domino/tandem processes.
- Development of unprecedented enantioselective variants of inter- and intramolecular Morita-Baylis-Hillman reaction.
- Various metal-catalyzed and metal-free organocatalytic approaches for the cyclopentannulation of arenes and heteroarenes.
- Enantioselective total synthesis of bioactive natural products and medicinally important compounds.

***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/dr-sripada-s-v-rama-sastry

Standing (from left): Uttam, Bara, Raju, Kaushalendra, Bishnu, Siddheshwar

Sitting (from left): Pinku, Shivangi, Ramasastry, Rajendra, Sonu, Atanu

**Selected Publications:**

**(1)** "Enantioselective organocatalytic intramolecular Morita-Baylis-Hillman (IMBH) reaction of dienones, and elaboration of the IMBH adducts to fluorenones" Satpathi, B.; Wagulde, S. V.; Ramasastry, S. S. V. *Chem. Comm.* **2017**, *53*, 8042.

**(2)** "One-Pot Multicatalytic Approaches for the Synthesis of Cyclohepta[*b*]indoles, Indolotropones, and Tetrahydrocarbazoles" Mishra, U. K.; Yadav, S.; Ramasastry, S. S. V. *J. Org. Chem.* **2017**, *82*, 6729.

**(3)** "Cyclopenta[*b*]annulation of Heteroarenes via Organocatalytic γ'[C($sp^3$)-H] Functionalization of Ynones" Raghu, M.; Grover, J.; Ramasastry, S. S. V. *Chem. Eur. J.* **2016**, *22*, 18316. [*Invited for a 'Frontispiece'*]

**(4)** "Synthesis of benzofurans via acid catalysed transacetalistion/ Fries-type O to C rearrangement/ Michael addition/ ring-opening aromatisation cascade of β -pyrones" Bankar, S. K.; Mathew, J.; Ramasastry, S. S. V. *Chem. Comm.* **2016**, *52*, 5569. [*Highlighted in 'Synfacts'*]

**(5)** "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.

**(6)** "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.

**(7)** "Synthesis of Polysubstituted Cyclopenta[*b*]indoles via Relay Gold(I)/Brønsted Acid Catalysis" Dhiman, S.; Ramasastry, S. S. V. *Chem. Commun.* **2015,** *51*,557**.** [*One of the most read articles during Nov-2014*]

**Samrat Ghosh**
**Assistant Professor**
E-mail: samrat@iisermohali.ac.in
Tel: +91 9779112516

# 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.

**Angshuman Roy Choudhury**
**Assistant Professor**
E-mail: angshurc@iisermohali.ac.in
Tel: +91 8054001404

# 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 (Ex. PhD student), 2010-2015 and Dr. Prasanta Bhowmik (Postdoc), 2015-till date, Hare Ram Yadav (PhD student), 2012-till date.

**Pharmaceutical Co-crystallization and their Applications:**

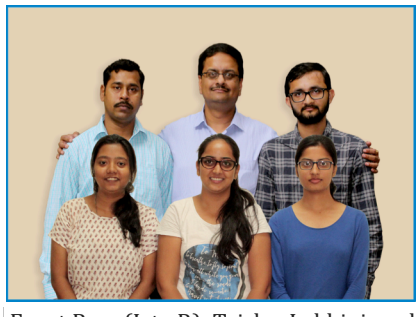
A number of known drugs suffer from various formulation difficulties related to their solubility, dissolution rate and thermal stability. We intend to develop novel drug composites to achieve better solubility and dissolution rates and higher thermal and storage stability of the well-known drugs through 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 (Ex. Project assistant), 2009-2013 and Ms. Indu Verma (MS student), 2013-14.

**Study of Weak Intermolecular Forces by Experimental and Theoretical Charge Density Analysis:**

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.



Front Row (L to R): Trisha, Labhini, and Anamika
Back Row (L to R): Prasanta, ARC, and Mayank

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

The structures of the compounds which are 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)** "The evaluation of the role of C—H···F hydrogen bonds in crystal altering the packing modes in the presence of strong hydrogen bond" Kaur, G.; Singh,S.; Sreekumar, A.; Choudhury, A. R., *J. Mol. Struct.*, **2016**, 1106, 154-169.

**(2)** "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.

**(3)** "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.

**(4)** "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.

**(5)** Study of Halogen-Mediated Weak Interactions in a Series of Halogen-Substituted Azobenzenes" Karanam, M.; Choudhury, A. R., *Cryst. Growth Des.* **2013**, 13, 4803.

**(6)** "Structural Landscape of Pure Enrofloxacin and Its Novel Salts: Enhanced Solubility for Better Pharmaceutical Applicability" Karanam, M.; Choudhury, A. R., *Cryst. Growth Des.* **2013**, *13*, 1626.

**K. R. Shamasundar**
**Assistant Professor**
E-mail: krsham@iisermohali.ac.in
Tel: +91 9915813389

# 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.**

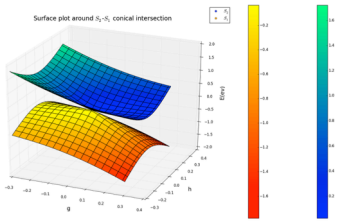
We have carried out a comparative study of charge symmetric dissociation of dications of $N_2$ and CO molecules, by computing potential energy curves for several states contributing to the experimentally observed KER pattern. Contributor: K. R. Shamasundar, Dr.Bhas Bapat and Dr.Amredra Pandey from PRL,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

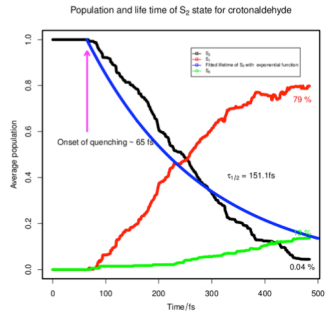
**Molecular Properties using Fock-space coupled-cluster methods.**

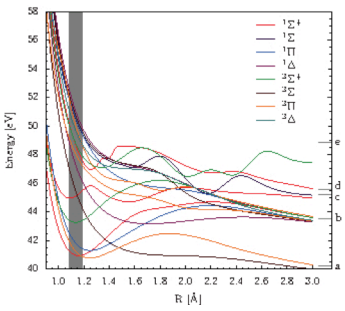
We are implementing a recently developed method for the analytic computation of molecular properties using a new formulation of FSCC theory. We expect this to be a cheap and useful alternative method to investigate electronic states near the Franck-Condon region. We have developed a new symbolic manipulation 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**
E-mail: sugumarv@iisermohali.ac.in
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

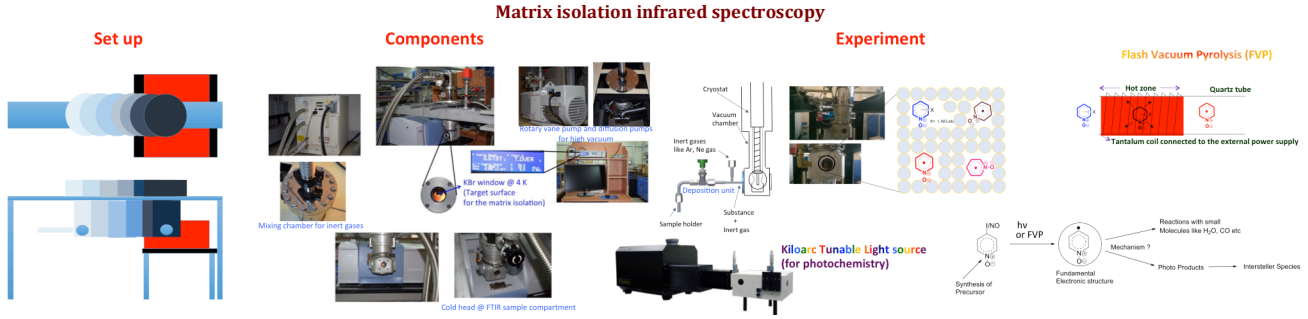
**Research Interests:**

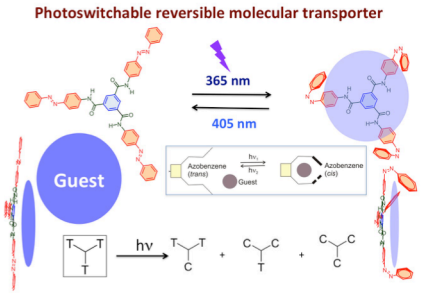
**Photoswitchable reversible molecular transporter: (**Funding : Start up & SERB, 2015 – 2018, EMR/2014/0000780**)**
Utilizing the concepts of photoswitching behavior, molecules containing multiple azobenzenes are designed and synthesized. They are expected to bind to the guest (drugs/ions etc.) as all-*cis* isomer and release it upon isomerization back to all-*trans*. Various spectroscopic techniques are the major tools. The long term goals are drug delivery and time - bound encapsulation.

**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)** "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.
**(2)** "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.
**(3)** "Rotational design of a room temperature molecular spin switch. The light-driven coordination induced spin state switch (LD-CISSS) approach" Marcel Dommaschk, Christian Schutt, Sugumar Venkataramani, Umasish Jana, Christain Nather, Frank D. Soennichsen, Rainer Herges, *Dalton Trans.*, **2014**, *43*, 17395-17405.




Group Members:

(From left): Himanshu Kumar, Ankit Somani (MS thesis), Ankit Gaur, Chitranjan Sah, Anjali Mahadevan, Sudha Devi, Virender Singh (MS theis), Surbhi Grewal, Pravesh Kumar, Anjali Srivastava, Debapriya Gupta, Mayank Saraswat

**Balanarayan P**
**Assistant Professor**
E-mail: balanarayan@iisermohali.ac.in
Tel: +91 8968216347

# Theoretical and Computational Chemistry

**Profile:**

**Ph.D** – 2008/University of Pune, Pune, Supervisor: Professor Shridhar R. Gadre
**Postdoc**–2009-2013/Technion, Haifa, Israel, Mentor: Professor Nimrod Moiseyev

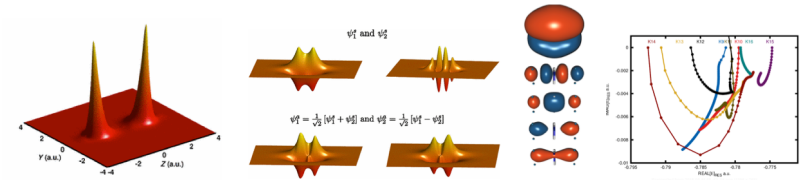
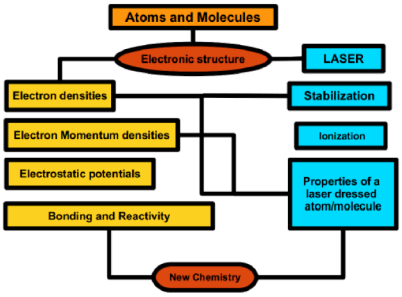


**Figure:** Laser dressed orbitals of sulfur atom and ammonia, complex scaling studies of helium atom

**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. A pictorial summary of our research interests is given in the figure above.

**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.

Funding : ~26 lakhs (DST-SERB-EMR Approved, 2015)

Contributors: Prashant

**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. There have been recent experiments by Krause *et al.* presenting the higher harmonic generation spectra for pyramidal ammonia cation. In our project we are currently probing how the planar geometry is realized in a CW laser and what are its experimental signatures. The laser dressed orbitals for planar ammonia are given the figure above.

**From the left/front:** Mishu, Alkit, Prashant, Naveen, Nitin, Prateek, Saurabh, Ashima, Gaganpreet, Bal Krishan, Balanarayan and Deepraj

**Life times of metastable electronic states:** Calculating lifetimes of metastable states using complex scaling methods is yet another area that we are working on. The current problems of interest for us are complex potential energy surfaces of dihydrogen anion and carbon monoxide anion.

**Properties of atoms and molecules and general computational chemistry**: The analysis of structure and properties atoms and molecules has been followed by Deep Raj Meena. Deep Raj Meena has been looking information entropies of position space and momentum space densities of laser dressed atoms.

**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.

**Sabyasachi Rakshit**
**Assistant Professor**
E-mail: srakshit@iisermohali.ac.in
Tel: +91 7837476759

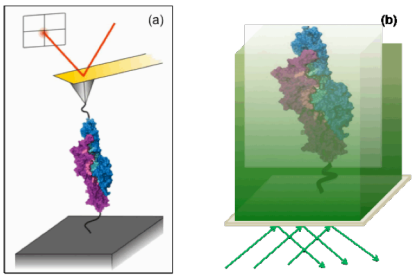
# Nanomechanics of Biomolecules

**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

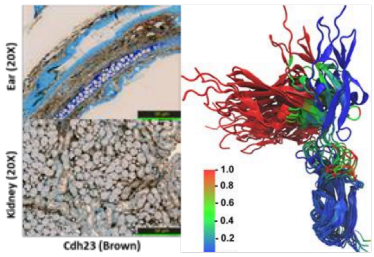
**Research Interests:**

**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.

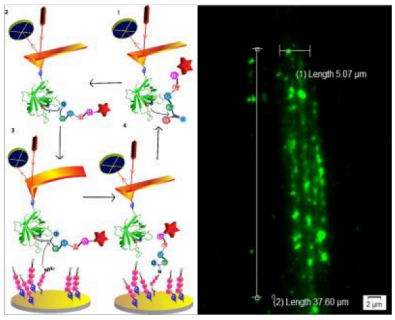
**Funding** : DBT-Wellcome Trust Intermediate Fellowship (Awarded, 2015)




**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)** "ESCORTing proteins directly from whole cell-lysate for single-molecule studies." Srinivasan, S., Hazra, J., Singaraju, G., Deb, D., Rakshit, S., *Anal. Biochem.* **2017**, 535, 35.
**(2)** "Resolving the molecular determinants of cadherin catch bond formation." Manibog, K., Li, H., Rakshit, S., Sivasankar, S., *Nat. Comm.* **2014**, 5, 3942.

Left,Back: Nisha, Gayathri, Sai, Jagadish, Left-Front: Surbhi, Amin, Sabyasachi, Malay and Anuj (!!)

**Arijit Kumar De**
**Assistant Professor**
E-mail: akde@iisermohali.ac.in
Tel: +91-172-229-3111

# Experiment (Ultrafast spectroscopy and Optical trapping) Theory (Analytical theory with numerical simulation)

## 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 are interested in developing novel time-resolved optical spectroscopic and microscopic tools to study a range of interesting chemical and biological phenomena in condensed phase.

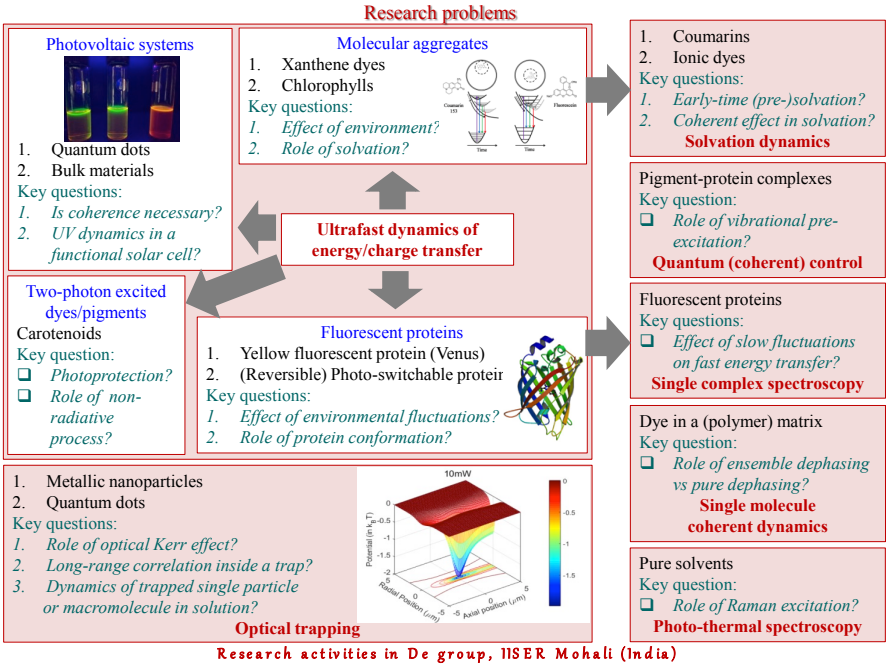
In particular, we are interested to study and, hopefully, control (?!) coherent energy/charge transfer dynamics within natural light harvesters (for example, photosynthetic pigment-protein complexes, fluorescent proteins) as well as their artificial analogs (for example, molecular aggregates, photovoltaic materials) both at the bulk/ensemble level (using femtosecond pump-probe and two- dimensional electronic spectroscopy) as well as at the single molecule/molecular-complex/particle level (using single-molecule spectroscopy) which are supported by theory.

We are also interested in understanding spatial organization of complex (biological) structures using fluorescence microscopes and understanding nano-scale optical forces using femtosecond laser tweezers. For the latter, we have developed an analytical theory including nonlinear optical effects and accurately estimated force/potential with numerical simulation.

The flowchart below depicts different research areas that are presently being pursued in our lab.

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)** "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 (2), 023856.
**(2)** "Theoretical investigation on optical Kerr effect in femtosecond laser trapping of dielectric microspheres" A. Devi and A. K. De, *Journal of Optics (IOP Publishing)*, **2017**, 19 (6), 065504.
**(3)** "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 (9), 21485.
**(4)** "Two-dimensional fluorescence-detected coherent spectroscopy with absolute phasing by confocal imaging of a dynamic grating and 27-step phase-cycling" A. K. De, D. Monahan, J. M. Dawlaty and G. R. Fleming, *Journal of Chemical Physics*, **2014**, 140, 194201.
**(5)** "Towards controlling molecular motions in fluorescence microscopy and optical trapping: a spatiotemporal approach" A. K. De and D. Goswami, *International Reviews in Physical Chemistry*, **2011**, 30, 275.

**Present group members:**
Front Row (R to L): Meghanad, Ajit, Pragya, Shaina, Pankaj and Arindam
Back Row (R to L): Yogita, Somrita, Shreya, Anita, Monika and AKDe
Missing: Samita

**Ujjal K. Gautam**
**Assistant Professor**
E-mail: ujjalgautam@iisermohali.ac.in
Tel: +91 7087649663

# Nanomaterials and Renewable Energy

**Profile:**

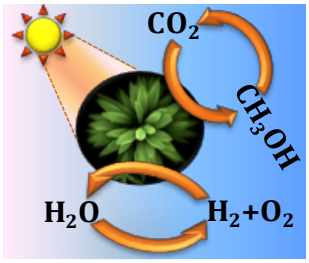
**Ph.D** – 1999-2006/Indian Institute of Science
**Postdoc**– 2006-08/National Institute for Materials Science, Tsukuba, Japan
**ICYS-Independent researcher**-2008-11
**Ramanujan Fellow** – 2011-14, JNCASR, Bangalore

**Research Interests:**

Our research works focus on synthesis and characterization of functional nanomaterials and their applications in 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:**

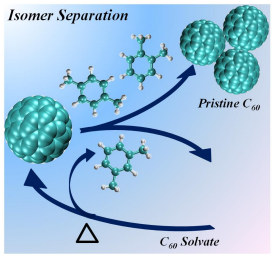
With the daily mean concentrations of atmospheric carbon dioxide having reached 400 parts-per-million for the first time in human history, the need for carbon-neutral alternatives to fossil fuel energy has never been more compelling. Nanomaterials with excellent activity, greater selectivity, and high stability. Their properties can be tuned by tailoring the size, shape, and morphology of the particular nanomaterial. In the *Nanomaterials and RenewableEnergy Laboratory*, weplan 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 energyharvesting, (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)** "Mechanochemical Synthesis of Free-Standing Platinum Nanosheets and Their Electrocatalytic Properties" M. Chhetri, M. Rana, B. Loukya, P. K. Patil, R. Datta, U. K. Gautam,*Adv. Mater.,* **2015**, 27, 4430.
**(2)** "$C_{60}$ 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.
**(3)** "Tuning the oxygen release temperature of metal peroxides over a wide range by formation of solidsolutions" S R. Lingampalli,D. Krishnan , R. Datta, U. K. Gautam,*Chem. Mater.*, **2014**, 26, 2720.

Group Members:

(From left): Dr. Moumita, Lipi Kaustav, Dr. Ujjal, Dr. Karthik, Dr. Arabindo and Sanjit

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

# Synthetic Inorganic, Organometallic, Catalysis

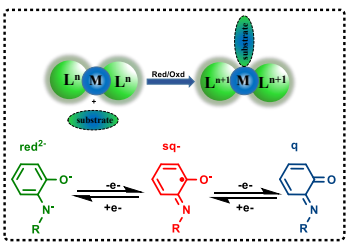
### Profile:

**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

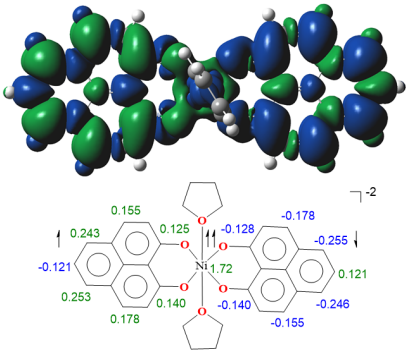
### Research Interests:

**(1) Redox-active ligand based metal complexes for catalysis and small molecule activation**

Redox active ligands (RAL) recently attracted tremendous research focus since base metal catalysis can be realized when RAL is electronically tuned with a 3d transition metal. The 3d transition metals are naturally inclined to perform one-electron chemistry in contrary to their heavier congeners, such as Pd, Pt, Rh, Ru etc. In principle, the RAL can be utilized as the reservoir or sink for redox equivalents and electrons can be supplied to the metal center on-demand. A proper electronic communication can help performing two-electron chemistry at the 3d- transition metal center, without promoting it to an unusual and unfavorable oxidation state. Parallel to this metal-based chemistry (borrowing electrons from RAL), ligand mediated radical chemistry to perform catalysis can also be envisaged. Our group will attempt to develop base metal catalysts using knowledge earned from electronic structure understanding by relevant spectroscopy and computations.

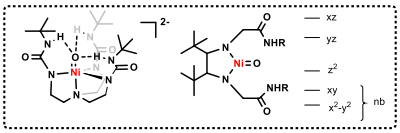



Recently, in collaboration with chemists in IISER Kolkata we have developed a nickel-based hydrosilylation catalyst which acts on the said principle. Ply is an odd alternant hydrocarbon and the highly delocalized backbone can accommodate electrons upon chemical or/and electrochemical reduction. Leveraging on this property, two electrons were donated externally (by potassium) and stored on the PLY backbone which triggers Si-H bond splitting chemistry. Shown below is the AF-coupled ground state of the catalyst and spin density.




**(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)** A New Strategy towards the Synthesis of a room-temperature Discotic Nematic Liquid Crystal by Employing Triphenylene and Pentaalkynylbenzene Units. Gupta, M.; Gupta S. P.; Rasna, M. V.; **Adhikari, D.**; Dhara, S.; Pal, S.K. *Chem. Commun.*, **2017**, *53*, 3014-3017.

**(2)** Cyclic (Alkyl)aminoCarbenes Based Iron Catalyst for the Regioselective Dimerization of Terminal Arylalkynes."Bhunia, M; Sahu, S. R.; Vijaykumar, G.; **Adhikari,D***.; Mandal, S. K. *Organometallics*, **2016**,*35*, 3775–3780.

**(3)** A Highly Efficient Base-Metal Catalyst: Chemoselective Reduction ofImines to Amines Using An Abnormal-NHC-Fe(0) Complex.Bhunia, M; Hota, P. K.; Vijaykumar, G.; **Adhikari,D**.; Mandal, S. K. *Organometallics*, **2016**,*35*, 2930–2937.

**(4)** Highly Active Carbene Potassium Complexes for the Ring-Opening Polymerization of Cyclic Esters"Bhunia, M; Vijaykumar, G.; **Adhikari,D***.;Mandal, S. K.* *Inorg. Chem.*,Under Review

**(5)** Intramolecular Ring-opening from a $CO_2$-derived Nucleophile as the Origin of Selectivity for 5-substituted Oxazolidinone from the(Salen)Cr-Catalyzed [Aziridine + $CO_2$] Coupling.**Adhikari, D.**; Miller, A. W.; Baik, M-H.; Nguyen, S. T. *Chem. Sci.*, **2015**, *6*, 1293-1300.

Group

**From Left:** Sonam, Dr. Adhikari, Amreen, Kirti.

**Sanchita Sengupta**
**Assistant Professor**
E-mail: sanchita@iisermohali.ac.in
Tel: +91 8217662891

# Organic Light Harvesting Materials

**Profile:**

**Ph.D** – 2006-11/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-May 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.

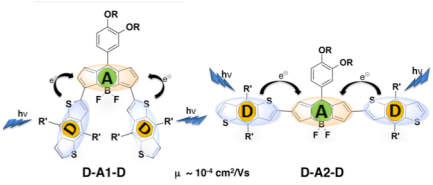



**Fig 1. Schematic representation of regioisomeric D-A-D systems with efficient PET and charge carrier mobilities.**

**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.

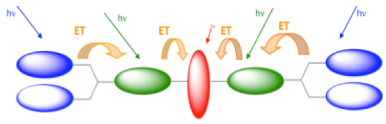


**Fig 2. Schematic representation of multichromophoric LH system for FRET.**

Eventual aim would be 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.

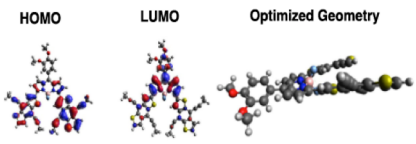



**Fig 3. DFT calculated frontier molecular orbitals (FMOs) and optimized geometry of a D-A-D triad.**

FRET and PET properties will be tuned based on DFT computed optical properties of separate donor and acceptor units.

**Selected Publications:**

**(1)** "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.
**(2)** "Tunable and highly efficient light-harvesting antenna systems based on 1, 7-perylene-3, 4,9, 10-tetracarboxylic acid derivatives." R. K. Dubey, D. Inan, **S. Sengupta**, E. J. R. Sudhölter, F. C. Grozema, W. F. Jager, *Chemical Science* **2016**, *7*, 3517-3532.
**(3)** "Highly Efficient Synthesis of Regioisomerically Pure 1,7-Dibromo Perylene-3,4,9,10-Tetracarboxylic Acid Derivatives" **S. Sengupta**, R. Dubey, R. Hoek, S. van Eeden, D. Gunbas, F. C. Grozema, E. Sudhölter, W. Jager, *J. Org. Chem.* **2014**, *79*, 6655–6662.
**(4)** "Chlorophyll J-Aggregates: From Bioinspired Dye Stacks to Nanotubes, Liquid Crystals and Biosupramolecular Electronics" **S. Sengupta**, F. Würthner, *Acc. Chem. Res.* **2013**, *46*, 2498–2512.
**(5)** "Biosupramolecular wires derived from tubular chlorophyll dye aggregates with exceptional charge transport properties" **S. Sengupta**, D. Ebeling, S. Patwardhan, X. Zhang, H. von Berlepsch, C. Böttcher, V. Stepanenko, S. Uemura, C. Hentschel, H. Fuchs, F. C. Grozema, L. D. A. Siebbeles, A. R. Holzwarth, L. Chi, F. Würthner, *Angew. Chem., Int. Ed.* **2012**, *51*, 6378–6382.

**Funding :**
1) IISER Mohali (Start up grant).
2) DST-INSPIRE Faculty Fellowship (Ongoing, 2013-18).
3) DST-SERI (Ongoing, 2015-18).

**Jino George**
**Assistant Professor**
E-mail: jgeorge@iisermohali.ac.in
Tel: +91 8146257106

# Strong Coupling Chemistry

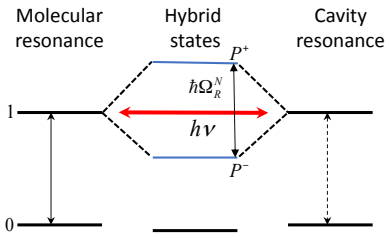
**Profile:**

**Ph.D** – 2006-12/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:**

**Light-matter interactions**



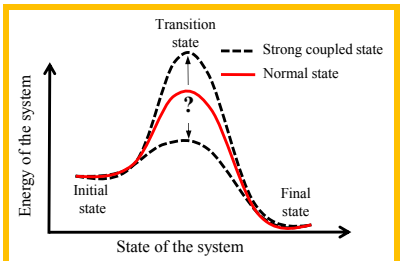

**Scheme 1**: Light-matter hybridization of a photon and a molecular state.

The chemical and physical properties of molecular materials depend on weak and strong matter-matter interaction of their constituents. For example, gaseous He-atoms turn into liquid at very low temperature due to weak London dispersion forces, whereas, strong electrostatic interactions of $Na^+$ and $Cl^-$ ions create an ionic crystal at room temperature. These interactions are operated by fluctuation of the electric field of the associated atom or molecule in the system. A similar scenario can be drawn in light-matter interactions in which a photon (light) interact with a two level molecular state (fluctuating electronic cloud) and modify their properties by weak or strong interactions.[1] As shown in the schematic above, under strong coupling (SC), the properties of the system are no longer purely those of the molecular constituents as they are modified by the appearance of new hybrid states generated by the *molecule – vacuum field* interactions. Coherence and tunability of energy levels are two other benefit of such hybridization. SC is typically achieved by placing an absorber in a resonant Fabry-Perot cavity under the right condition.

Our group activities can be broadly divided under the umbrella of chemistry (*STRONG*$^{chem}$) and material science (*STRONG*$^{matter}$). Two of the main projects are mentioned below.

**Project 1: Chemistry under strong coupling (*STRONG*$^{chem}$)**

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 (Scheme 2). Very recently we experimentally proved that a ground state chemical reaction can be modified by coupling molecular vibrations to vacuum electromagnetic field or zero point energy of a resonant IR micro-fluidic cavity.[2] The focus of the current study is to understand in depth the influence of vibrational strong coupling (VSC) on the chemical reactivity of molecules to determine the underlying principles, to make it as a novel and useful tool for chemists.




**Scheme 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: Light-matter strong coupling for material science (*STRONG*$^{matter}$)**

In this project, efforts will be made to study electron/energy transfer processes mediated by extended nature of the polaritonic states of electronically and vibrationally coupled systems.[3] Here, more emphasis will be given for improving the efficiency of transport in molecular materials, both electron and energy transfer rates via the polaritonic states. As mentioned above, these states can be modified in terms of their energy levels and understanding the dynamics of energy migration in such hybrid delocalized systems are of potential interest in light harvesting and biological systems.


**Scheme 3**: Coherent polaritonic states

**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. Chemie 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.

**Monika Sharma**
**Inspire Faculty**
E-mail: mnsharma@iisermohali.ac.in
Tel: +91 7087543458

# 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:**

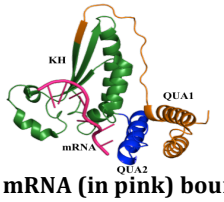
I am interested in application of computational methods to study the conformational dynamics of the biomolecules and interactions among them. I primarily uses molecular dynamics as principal tools for the theoretical study of biological molecules and their complexes. Atomistic molecular dynamics (MD) simulations present a convenient way to derive information by sampling dynamic molecular processes and can provide atomic level description of structural stability and function which are difficult to be obtained from the experimental studies. 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. I have used combinations of these techniques to investigate the conformational dynamics of proteins, nucleic acids, and their complexes as well.

Currently, I am involved in these following topics:

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

Signal Transducer and Activator of RNA (STAR) proteins specifically, SF-1, GLD-1, and QKI proteins have been shown to function in pre-mRNA splicing, mRNA export, mRNA stability, and protein translation. These have critical implications in many cellular processes. They have also been reported to be associated with numerous human pathologies like cancers and neurological disorders such as human inherited ataxia, multiple sclerosis, or schizophrenia. Theoretical studies are being used to investigate the molecular basis of recognition, binding, and regulation of mRNA by this family of transcriptional regulators by employing molecular dynamics and enhanced sampling techniques.

In addition, this work methodology can act as a protocol to understand the underlying principles of RNA binding to various categories of RNA binding proteins (RBPs), and the comparative analyses will address how RBPs function as part of multi-molecular assemblies that constitute the structural and functional units of gene expression?

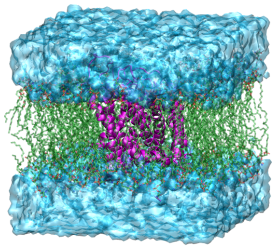



**mRNA (in pink) bound GLD-1**

Funding: INSPIRE, DST (Support money and research grant for 5 years)

**Other areas of interest**

The other areas of my research interests are molecular modeling of proteins involving structure prediction for further mapping with their function, and investigating stabilization of RNA structure via tertiary interactions.



**Modeled transmembrane protein (violet) embedded in lipid bilayer (green)**

**Selected Publications:**

**(1)** "Insights into the molecular basis for substrate binding and specificity of the fungal cystine transporter CgCYN1" A.A.Deshpande, M. Sharma, and A.K. Bachhawat. *BBA-Biomembranes*, **2017,** *in press.*

**(2)** "Long-range signaling in MutS and MSH homologs via switching of dynamic communication pathways". B. Wang, J. Francis, M. Sharma, S.M. Law, A.V. Predeus, and M. Feig. *PLoS Comput. Biol.*, **2016**, 12(10): e1005159.

**(3)**"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. *Biochem. J.*, **2016,** 473(15), 2369-2382.

**(4)** "Differential Mismatch Recognition Specificities of Eukaryotic MutS Homologs, MutSα and MutSβ." M. Sharma, A. V. Predeus, N. Kovacs, and M.Feig. *Biophys. J.*, **2014**, 106, 2483.

**(5)** "A designed conformational shift to control protein binding specificity." S. Michielssens, J. H. Peters, D.Ban, S. Pratihar, D. Seeliger, M. Sharma, K.Giller, T.M. Sabo, S. Becker, D. Lee, C. Griesinger, Bert L. de Groot. *Angewadte Chemie*, **2014**, 53(9), 10367.

**(6)** "Conformational preferences of DNA in reduced dielectric environment.". A. Yildirim, M. Sharma, B. Varner, L. Fang and M. Feig. *J. Phys. Chem. B.*, 118(37), **2014**, 10874-10881.

**Debrina Jana**
**Inspire Faculty**
E-mail: debrina@iisermohali.ac.in
Tel: +91 7744029918

# Chemistry at Nanoscale

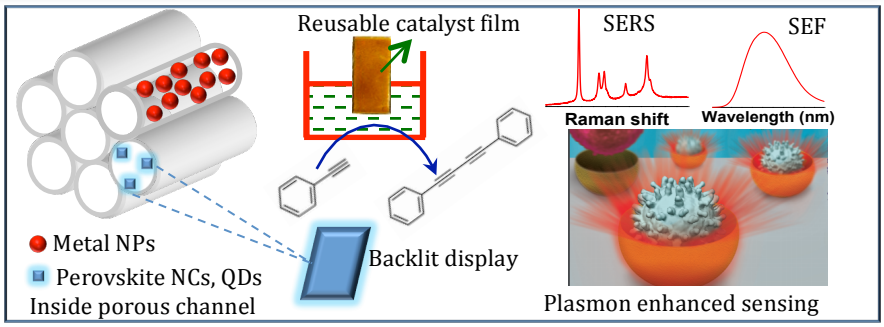
**Profile:**

**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:

**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, perovskite etc. inside the mesoporous channel keeping in view the goal to fabricate advanced materials for optoelectronic, catalytic applications.




**Controlled synthesis and assembly of metallic nanoparticles:**
We are interested in designing strategies for synthesizing nanomaterials with controllable size, shape and composition and assembling them in a predetermined fashion (Application: heterogeneous catalysis, sensing and bio-targeting).

**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.

Funding: DST (Ongoing, 2016-2021), Contributors: Daimiota Takhellambam, Shikha Bhateja

Group members: (From left) Daimiota, Debrina, Shikha

**Selected Publications:**

**(1)** "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.
**(2)** "Capping agent-free gold nanostars show greatly increased versatility and sensitivity for biosensing" Jana, D., Matti, C., He, J., Sagle, L., *Anal. Chem.,* **2015**, 7, 3964.
**(3)** "A Facile Synthesis of Cubic (Im3m) Alumina Films on Glass with Potential Catalytic Activity" Mitra, A., Jana, D., De, G., *Chem. Commun.,* **2012**, 48, 3333.
**(4)** "High Raman enhancing shape-tunable Ag nanoplates in alumina: A reliable and efficient SERS technique" Jana, D., Mandal, A., De, G., *ACS Appl. Mater. Interfaces,* **2012**, 4, 3330.
**(5)** "Spontaneous generation and shape conversion of silver nanoparticles in alumina sol, and shaped silver nanoparticle incorporated alumina films" Jana, D., De, G., *J. Mater. Chem.,* **2011**, 21, 6072.
**(6)** "Tunable Au-Ag Nanobowl Arrays For Size-Selective Plasmonic Biosensing" Jana, D., Lehnhoff, E., Bruzas, I., Robinson, J., Lum, W., Sagle, L., *Analyst*, **2016**, 141, 4870.

**Bimalendu Adhikari**
**Inspire Faculty**
E-mail: badhikari@iisermohali.ac.in
Tel: +91 9933898711

# Molecules to Materials

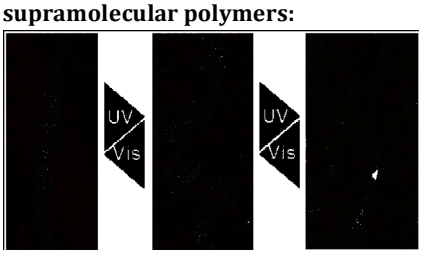
**Profile:**

**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:**

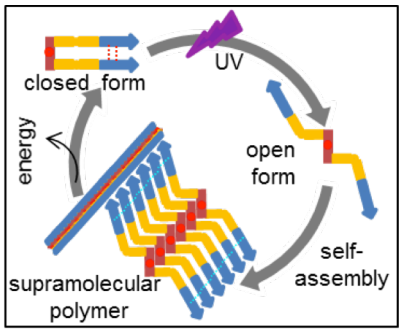
Supramolecular Polymer, Dissipative and Non-dissipative Assemblies, Gels, Bioorganic Chemistry, Peptides, Nanomaterials

**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

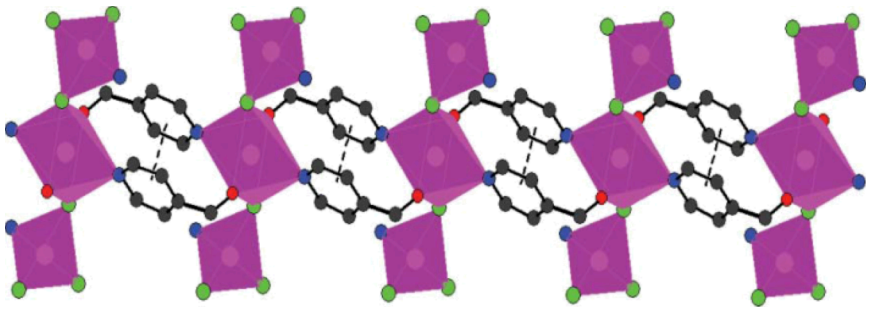
Funding: DST-INSPIRE (ongoing, 2016-till date)
Contributors: Aleena Thomas (Graduate student), Geethu Venugopal, Joyal Davis (Master students)

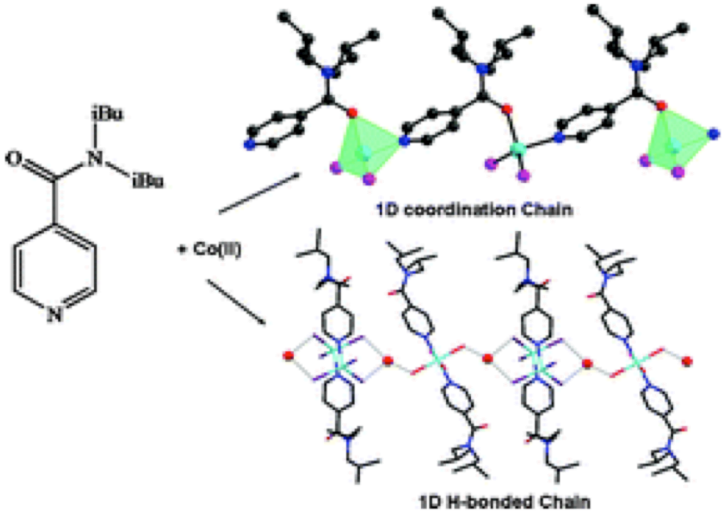
**Selected Publications:**

**(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.

**Ramesh Kapoor**
**Professor**
E-mail: rkapoor@iisermohali.ac.in
Tel: +91 9815247070

# Former Faculty






**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.

# Visiting Faculty

**Dr. J. Narasimha Moorthi**

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

**Dr. Ram Mohan**

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

**Dr. Michael Baer**

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

**Dr. Mangala Sunder Krishnan**

Professor
Department of Chemistry
IIT Madras, Chennai – 600 036
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 (Convenor) and all other DCS members in various capacities.

**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

# Awards/Honours/Achievements/Recognitions

**Faculty**

- Rama Sastry Sripada has received the Chemical Research Society of India (CRSI) Bronze Medal for the year 2018.
- S. V. Rama Sastry Sripada has received Thieme Chemistry Journal's Award 2017 [Chosen by the Editorial Boards of Synlett, Synthesis, and Synfacts]
- Arijit Kumar De has received DST travel fellowship to attend Gordon Conference on "Quantum Control of Light and Matter", USA, 2017. (Application No. - ITS/Off-502/2017-18)
- Arijit Kumar De has received INSA travel fellowship to attend Gordon Conference on "Quantum Control of Light and Matter", USA, 2017. (INSA travel Grant No. SS/INSA/2017/758)
- Arijit Kumar De has received SERB, DST Early Career Research Award, 2016. (Grant No: ECR/2016/000467)
- S. 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) in 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 Ramchandran received the best teacher's award from IISER Mohali (2013)
- Santanu Kumar Pal has received DAE Young Scientist Research Award (2012)
- Sanjay Singh was elected as Young Associate of the Indian Academy of Sciences in Bangalore (2009-2013)
- Samrat Mukhopadhyay has been selected as a Young Associate of the Indian Academy of Sciences. (2009-2013)
- Samrat Mukhopadhyay has been invited to contribute profile annual issue of 'Who's who in Fluorescence' (Published by Springer. Editor: Chris D. Geddes, University of Maryland Baltimore County). (2009)

# Awards/Honours/Achievements/Recognitions

**Sudents & Postdocs/RA's**

- 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 (PhD stdent/SS group) attended the 11th International Symposium on Macrocyclic and Supramolecular Chemistry, 10-14 July, 2016. Travel support by IISER Mohali

- Mr. Deependra Bawari (PhD stdent/SS group) received International Travel award from DST-SERB to attend the 12th International Symposium on Macrocyclic and Supramolecular Chemistry, 02-06 July, 2017 (Cambridge, London (UK).

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

- Dr. Anamika Mukhopadhyay (Postdoc/Prof. K. S. Viswanthan's group) has received CSIR Pool Scientist award. (2015)

- Ms. Indu Verma (PhD Student/SK Pal Group) won The Dewan Jawahar Lal Nayar Memorial prize at the 21st National Conference on Liquid Crystals (NCLC) held at VSSD College, CSJM University, Kanpur and received best poster award. (2014)

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

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

- Dr. Sadhika Khullar (Graduate student) has defended her thesis entitled "Metal Organic Coordination Networks Comprised of Divalent Metal Centers and Multiatom Carboxylate Linkers" under the supervision of Dr. Sanjay Mandal and graduated as a first doctoral student from the department . (2013)

- Ms. Shilpa Setia (Graduate student/SKPal group) won The Dewan Jawahar Lal Nayar Memorial prize at the 20th National Conference on Liquid Crystals (NCLC) (est poster presentation). (2013)

- Ms. Sumyra Sidiq (Graduate student/SKP group) has been adjudged the best in poster presentation and won The Dewan Jawahar Lal Nayar Memorial prize at the 19th NCLC held at the Thapar University, Patiala. (2012)

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

# Awards/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) |
| 16 | Anjana/MS15 | CUSAT, Cochin | 2016 | VSRP fellowship |
| 17 | Priyanka Bansal/MS13 | Indiana University, USA | 2017 | Summer Internship |
| 18 | Divita Gupta/MS13 | University of Rennes 1, France | 2017 | Summer Internship |
| 19 | Rishabh Gupta/MS14 | TIFR Hyderabad | 2017 | VSRP fellowship |
| 20 | Himanshi Singh/MS14 | IISER, Pune | 2017 | SSPC fellowship |
| 21 | Vidhyalakshmi.S/MS14 | TIFR , Hyderabad | 2017 | VSRP fellowship |
| 22 | Parth Raval /MS14 | BARC, Mumbai | 2017 | Institute fellowship |
| 23 | Anjana/MS15 | TIFR Hyderabad | 2017 | VSRP Fellowship |
| 24 | Vaibhav Pal/MS15 | Centre for Nano and Soft Matter Sciences (CeNS),Bengaluru | 2017 | ROIS |

# 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

**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 Current Position

**Chemistry major (MS) students**

| Name | Batch | Current Position |
|---|---|---|
| Amita Agarwal | MS07 | Process Researcher at Shell India |
| Mrinal Shekhar | MS07 | PhD at University of Illinois at Urbana–Champaign |
| Shalender Jain | MS07 | Lecturer at Govt. College Haryana |
| Gaurav Kumar | MS08 | PhD at University of Southern California, USA |
| Kapil Dave | MS08 | PhD at University of Illinois, Urbana-Champaign, USA |
| Asif Iqbal | MS08 | PhD at Aarhus university, Denmark and TIFR Mumbai |
| Vinod Kumar | MS08 | PhD at IISER Mohali |
| Sumit Mittal | MS08 | PhD at Max Planck Institute for Coal Research, Germany |
| Deepansh Shrivastava | MS08 | PhD at Ohio State university, USA |
| Manish Pareek | MS08 | PhD at TU Berlin, Germany |
| Mariyam Fatima | MS09 | PhD at Max Planck Institute of Structure and Dynamics of Materials, Germany |
| Nishtha Agarwal | MS09 | PhD at Cardiff Catalysis Institute, UK |
| Deepak Verma | MS09 | PhD at University of Southern California, USA |
| Karan Pratap Singh Yadav | MS09 | MBA from IIM Calcutta, India |
| Jyoti Saini | MS09 | PhD at IISER-Mohali, India |
| Indu Verma | MS09 | PhD at IISER-Mohali, India |
| Priyanka Dogra | MS09 | PhD at IISER-Mohali, India |
| Agastya P. Bhati | MS09 | PhD at University College London, UK |
| Aditya Jhajharia | MS09 | PhD at École Normale Supérieure, Paris |
| Gaurav Verma | MS09 | PhD at University of South Florida, USA |
| Yash Maurya | MS09 | MBA from School of Petroleum Management, Gandhinagar |
| Sudeep Maheshwari | MS09 | PhD at TU Delft, Netherlands |
| Shiv Charan Dudi | MS09 | Lecturer at Allen Career Institute, Kota, India |
| D. Jeiyendira Pradeep | MS10 | PhD at TIFR, Mumbai/University of Lille 1, France |
| Vipin T.Raj | MS10 | Research Internship at IISER Thiruvananthapuram, India |
| Anubhuti Singh | MS10 | Project position at IISER Mohali |
| Ravi Ranjan | MS10 | Job at Azim Premji foundation |
| Bharti Kumari | MS10 | PhD at TIFR Mumbai, India |
| Piyush Mishra | MS10 | PhD at Purdue University, USA |
| Pratip Chakraborty | MS10 | PhD at Temple University, USA |
| Jagadish Prasad Hazra | MS10 | Project position 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 UNSW Canberra, Australia |
| Aneeshma Peter | MS10 | PhD at University of Quebec, Trois riveres, Canada |
| Arya J. S. | MS10 | PhD at NIIST, Trivandrum |
| Harshita Pawar | MS10 | PhD at IISER Mohali |
| Haseeb Hakkim | MS10 | PhD at IISER Mohali |
| Raut Akshay Hemant | MS10 | PhD at Ruhr University of Bochum, Germany |
| Rupali Chawla | MS10 | Research Internship at IIT Delhi, India |
| Prerna Paliwal | MS10 | PhD at Weizmann Institute of Science, Israel |
| Prashant Singh | MS10 | Research Internship at IISER Mohali, India |
| Rajat Garg | MS10 | Research Internship at IISER Mohali, India |
| Akhil V. Gopal | MS10 | PhD at IISER Kolkata |
| Shweta Sreenivasan | MS11 | PhD at Massachusetts Institute of Technology |
| Nakul Teke | MS11 | PhD programme at Virginia Tech, Virginia |
| Srijit Mukherjee | MS11 | PhD programme at University of Colarado, Boulder |
| Justin K. Thomas | MS11 | PhD programme at Ohio state University, Columbus |
| Lakshmi Bhai N. V. | MS11 | PhD programme at Ohio state University, Columbus |
| Manisha | MS11 | PhD at Massachussets University, Amherst |
| Sai Kumar Gobilla | MS11 | PhD programme at Technische Universitat, Munich |

# Alumni Current Position

**Chemistry major (MS) students**

| Name | Batch | Current Position |
|---|---|---|
| Shruthi Mohan | MS11 | PhD at University of Chicago |
| Jopaul Mathew | MS11 | PhD programme at Virginia Tech |
| Sabari | MS11 | PhD at IISER Mohali |
| Abhinay Vardhan | MS11 | PhD at IISER Mohali |
| Sandhya | MS11 | PhD at University of Otago, New Zealand |
| Anjali Mahadevan | MS11 | PhD at IISER Mohali |
| Athira T. John | MS11 | PhD at IISER Trivandrum |
| Aman Kumar Bhonsle | MS11 | PhD at CSIR IIP, Dehradun |
| Vaishali Vardhan | MS11 | PhD at Forschungszentrum Jülich |
| Neeru Mittal | MS12 | PhD at ETH Zurich |
| Aayush | MS12 | PhD at Purdue University |
| Satavisa Jana | MS12 | PhD at UCSD, California San Diego |
| Bhupendra Goswami | MS12 | PhD at Karlsruhe institute of Technology, Germany |
| Ankit | MS12 | PhD at IISER Mohali |
| Aleena Anna Thomas | MS12 | PhD at IISER Mohali |
| Mushir Ul Hassan | MS12 | PhD at Temple University |
| Anuj Pennathur | MS12 | PhD at University of Southern California |
| Anirudh CR | MS12 | PhD at Michigan State University |
| Mustafa Iqbal | MS12 | PhD at IISER Mohali |
| Ravi Ranjan | MS12 | PhD at University of Illinois, Chicago |
| Mohammed Shabin | MS12 | Project assistant, IISER M |
| Sruthy Chandy | MS12 | PhD at Indiana University, Bloomington |

**Former Ph. D Students**

| Name | Year of completion (Ph. D Supervisor) and Current Position |
|---|---|
| Dr. Neha Jain (Bio PhD) | 2013 (Dr. Samrat Mukhopadhyay), Postdoc at University of Michigan, USA |
| Dr. Sadhika Kullar | 2013 (Prof. Sanjay Mandal), Assistant Professor, DAV University, Jalandhar |
| Dr. Gurpreet Kaur | 2015 (Dr. Angshuman Roy Choudhury), Assistant Professor, DAV University, Jalandhar |
| Dr. Navnita Kumar | 2015 (Prof. Sanjay Mandal), Assistant Professor, S.D. College, Chandigarh |
| Dr. Zeba Qadri | 2015 (Dr. Ramesh Ramachandran) |
| Dr. Shilpa Setia | 2015 (Dr. Santanu Kumar Pal), Assistant Professor Bhag Singh Khalsa College for Women Abohar, Punjab |
| Dr. Sumyra Sidiq | 2015 (Dr. Santanu Kumar Pal), Assistant Professor, Govt. Degree College for Women, Govt of J & K |
| 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. Shruti Arya | 2017 (Dr. Samrat Mukhopadhyay), Will be joining for postdoc at the University of California Santa Barbara in July 2017. |
| Dr. Seema Rani | 2016 (Dr. S. V. Rama Sastry Sripada), Postdoc at Friederich 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. |
| Dr. Vadla Rajkumar | 2016 (Dr. S. Arulananda Babu), at GVK BioSciences, Hyderabad |
| Dr. Chennakesava Reddy | 2016 (Dr. S. Arulananda Babu), Post-Doc with Dr. R. G. Bhat, IISER, Pune. |
| Dr. Naveen | 2017 (Dr. S. Arulananda Babu), Wiezmann Institute of Science, Israel |
| Dr. Kuldeep Jaiswal | 2016 (Dr. Sanjay Singh), working at Nankai University, China as a Post-doctoral fellow. |
| Dr. Billa Prasanth | 2015 (Dr. Sanjay Singh), Postdoc at University of Bonn. |
| Dr. B. T. Ramanjaneyulu | 2016 (Dr. R. Vijaya Anand), Postdoctoral Fellow at POSTECH, South Korea |
| Dr. Virsinha Venkat Reddy | 2017 (Dr. R. Vijaya Anand), Postdoctoral Fellow at the University of Cape Town, South Africa |
| Dr. Panjab B. Arde | 2017 (Dr. R. Vijaya Anand) |
| Dr. Ramarao | 2017 (Dr. S. Arulananda Babu), Postdoc position offered at University of Texas San Antanio |
| Dr. Maumita Rana | 2017 (Dr. Ujjal K. Gautam) |
| Dr. Hare Ram Yadav | 2017 (Dr. Angshuman Roy Choudhury), Assistant Professor at SRM University, Lucknow |

# 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 |
|---|---|---|
| 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 |
| CHM307 | Electrochemistry and ionic equilibria | 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 |

# Publications

**2017**

1. Naveen; **Babu, S. A.,** "Exploitation of Intramolecular Glaser–Eglinton–Hay Macrocyclization for the Synthesis of New Classes of Optically Active Aza-Oxo-Thia Polyether Macrocycles from Amino Alcohol Building Blocks" *Synlett*, **2017**, *28*, 253.
2. Sankar, R.; **Babu, S. A.,** "Construction of tertiary amides: Ni (II)-catalyzed N-arylation of secondary acyclic amides (2-picolinamides) with aryl halides" *Asian J. Org. Chem.*, **2017**, *6*, 269.
3. Parella, R.; **Babu, S. A.,** "Pd (II)-Catalyzed, Picolinamide-Assisted, Z-Selective γ-Arylation of Allylamines to Construct Z-Cinnamylamines" *J. Org. Chem.*, **2017**, 82, 6550.
4. Parella, R.; **Babu, S. A.,** "Pd (II)-Catalyzed Arylation and Intramolecular Amidation of γ-C (sp3)-H Bonds: En Route To Arylheteroarylmethane and Pyrrolidone-Ring Annulated Furan/Thiophene Scaffolds" *J. Org. Chem.*, **2017**, 82, 7123.
5. **De, A. K.**, "Addressing Key Issues in *Photosynthetic Sunlight Harvesting By Utilizing Coherence: A Perspective*", *Open Acc. J. Photoen.***2017**, *1 (1)*, 00005.
6. Devi, A.; Dhamija, S.; **De, A. K.,** "Optical trapping with femtosecond laser pulses" *Proc. SPIE,* **2017**, 10347, 1034737 (1 – 5). http://dx.doi.org/10.1117/12.2273839
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# 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**

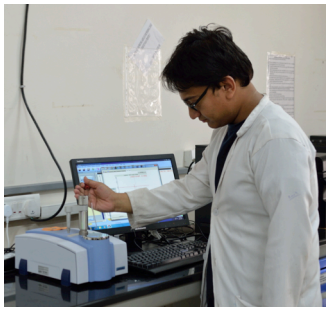
# The People

**MS13 and Integrated PhD 2015 batch Students**

**MS14 and Integrated PhD 2016 batch Students**

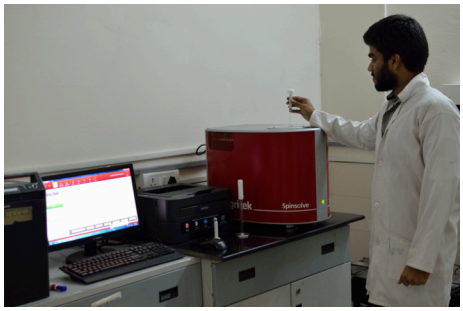
**MS15 and Integrated PhD 2017 batch Students**

# Glimpses from the Lab



The new miniaturized Bruker Alpha FT-IR spectrometer

Leco TruSPEC CHNS analyzer



Magritek Spinsolve benchtop NMR spectrometer

Lab assistants: (L to R) Mangat Ram, Ganesh Lal Meena, Satwinder, Prahlad Singh, Khem Bahadur, Chetan Kumar Gaur (Not in the picture) and Triveni Shanker

**Contact:**
Department of Chemical Sciences
Indian Institute of Science Education and Research Mohali
Sector – 81, SAS Nagar, Manauli
Punjab – 140 306, INDIA
Web: www.iisermohali.ac.in