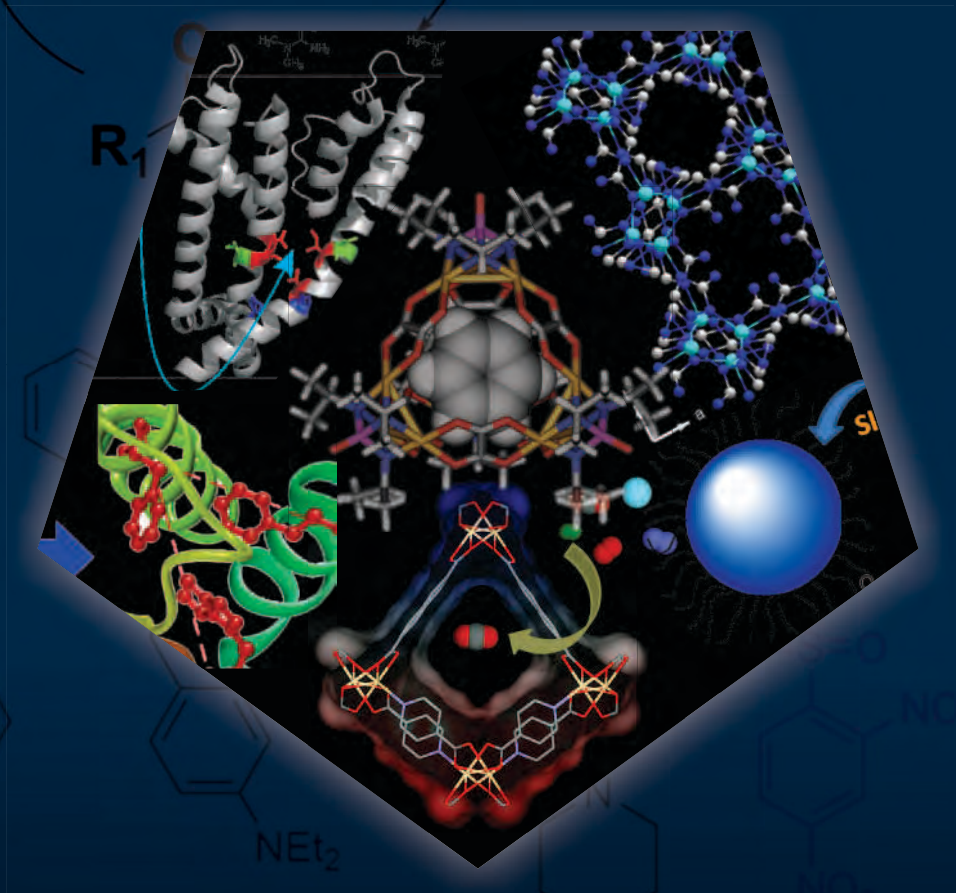
IISER PUNE

Chemistry @ IISER Pune

2006-2014



Indian Institute of Science Education and Research (IISER) Pune

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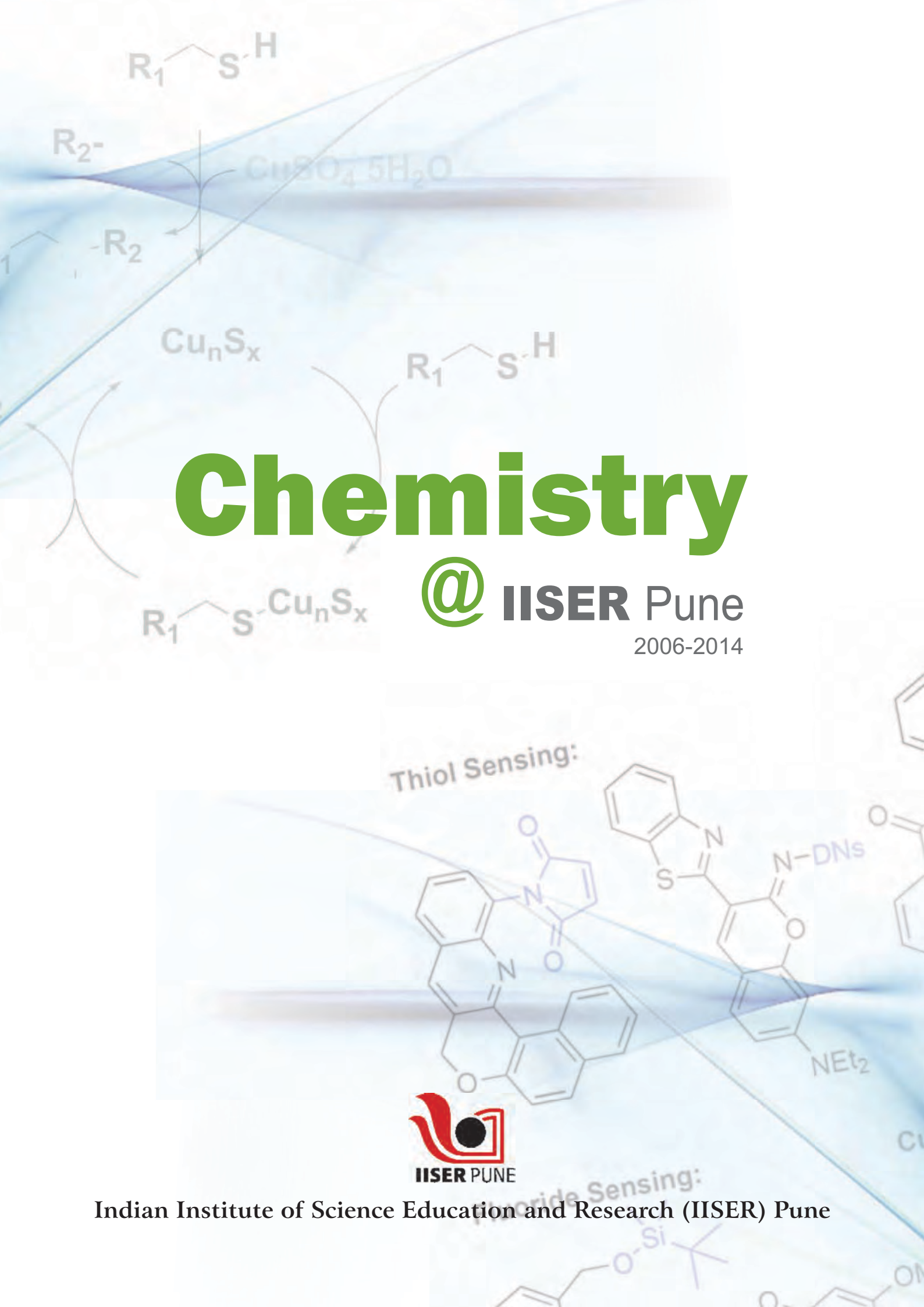

IISER PUNE

Indian Institute of Science Education and Research (IISER) Pune

Foreword

I have great pleasure in presenting the book "Chemistry @ IISER Pune 2006-2014" which chronicles the activities of the Chemistry Program at IISER Pune since the inception of the Institute in 2006. The chemistry teaching which started with general chemistry in semester of August 2006 in a modest way at the level of 1st year BS, has now expanded with a range of courses encompassing not only the basic four pillars – inorganic, organic, theoretical and physical – but also into the interdisciplinary areas of chemical biology, material science, polymer chemistry, spectroscopy and nanoscience. The teaching of various courses is integrated with the development of practical skills in laboratory, which is so essential in chemistry and fused to a complete one-year research programme in 5th year. It is gratifying to see that several research publications are emanating from UG research. Students have the option of taking up a UG research project not only at IISER Pune but also at other research Institutes in India, some abroad, and in industry as well. The aim of chemistry@iiserpune is to train students UG students in the breadth, depth and impart research experience before they graduate. In 2014, the BS-MS chemistry programme of the Institute was accredited by the Royal Society of Chemistry, UK – the first Institute in India to receive such recognition and this signifies the international equivalence of our BS-MS course.

The Institute started enrolling students in year 2007-2008 right from the day the first faculty member joined. At present, there are 163 PhD students in Chemistry (more than 40% of the total IISER Pune PhD students) and 11 have already received their PhD degrees till December 2014. Recently Institute post-doctoral programme in chemistry was introduced and 5 fellows have joined the programme.

In 2008, a small research laboratory to accommodate 20-25 students was established in the transit campus in Sai Trinity building, where more than 10 faculty members shared laboratory with active research under limited and trying conditions, without any sense of temporariness sinking. Even in the transit lab, high end instrumentation such as jet spectrometer coupled with TOF, High performance computer, 400 and 500 MHz NMR / MALDi Mass Spectrometer / single crystal X-ray diffractometer / analytical facilities (UV, fluorescence, CD, HPLC, GC etc) were immediately set-up. This was greatly helpful for the initial research and resulted in quick publications within the first two years and enabled attracting good faculty. The Institute practices high ethical and safety standards in the laboratories. Several national and international chemistry conferences that were organized brought in excellent scientists (Jean-Marie Lehn, George Whitesides, C.N.R. Rao, to name a few) and visitors, providing immediate motivation, scientific benefit and exposure to faculty and students. It was also gratifying to see that working under these conditions, some of the faculty received peer national recognition as well.

In 2011, the chemistry laboratory was the first one to move into the main campus into the Mendeleev block that housed 20 faculty offices and 4 large laboratories accommodating 120 PhD students and a dedicated instrument laboratory and modern chemical and solvent storage facilities. All visitors immediately noticed the design of labs incorporating all safety features. This greatly accelerated the output of the research programme in terms of quality of publication. The number of faculty members increased and the facilities allowed in-house fabrication of terahertz, femtosecond fluorescence and laser Raman spectrometers along with establishing biology labs to carry out immediate activity testing. For the last 3 years, Mendeleev provided the major buzz of chemistry research and the performance culminated in the recognition award of DST-FIST level II fund to acquire a 600 MHz NMR spectrometer, AFM and microfocus X-ray diffractometer.

Finally, October-2014 saw the shifting of major chemistry laboratories to the main building which now houses fully equipped wet and instrument labs, custom designed by each faculty member to their research needs. The Mendeleev block continues to provide extra lab space for all UG teaching laboratories and some research facilities. It is a matter of great satisfaction to the faculty members and students that they are now in their own independent laboratories and look forward to accelerated research work.

I should place on record the patience of all chemistry faculty members for bearing the inconveniences of temporary lab and office arrangements and repeated relocation of labs. None of these have dampened their spirit and they have without excuses continued to perform well. They are all acutely aware of the future science challenges ahead: how to advance and sustain the IISER Pune chemistry programme (teaching and research) amongst the best in the world. We know that we have miles to go before we realize this dream.

This brochure has been prepared as the performance report of the chemistry programme for the duration 2006-2014 for submission to the review committee and to record all the achievements so far.

As we enter 2015, I wish all the faculty and students well in their new laboratories.

Krishna N. Ganesh
Director and Discipline Co-ordinator, Chemistry (2006 – present)

January 7, 2015

Institutional Review and Scientific Advisory Committee (IRSAC)

for the Chemistry Programme at IISER Pune, India

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Fellow of Trinity College
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E-Mail: akc30@cam.ac.uk
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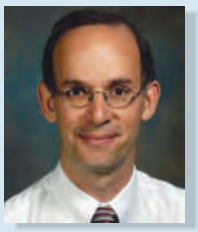
E-Mail: babu@chemistry.ohio-state.edu
https://chemistry.osu.edu/~babu/



Prof. M.G. Finn
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Contents

Faculty Profile

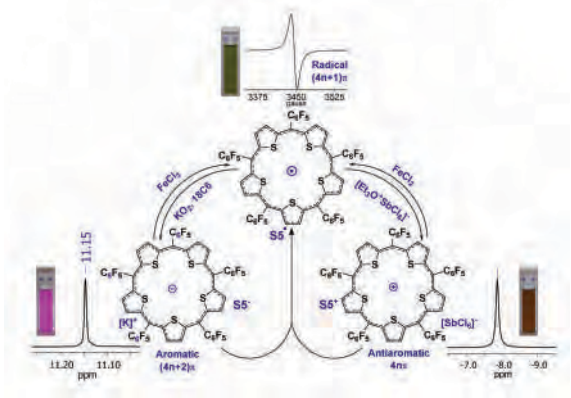
V. G. ANAND

Associate Professor

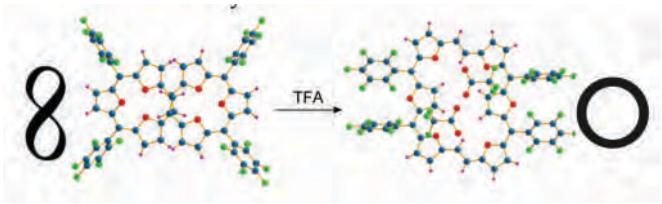
Ph.D.: Indian Institute of Technology, Kanpur, India
Post-doc.: JSPS Fellow, Kyoto University, Kyoto, Japan
Previous position: Scientist-C, NIIST (CSIR), Thiruvananthapuram
Assistant Professor: June 2007 – January 2013, IISER-Pune
Associate Professor: January 2013 – Present date, IISER-Pune
Email: vg.anand@iiserpune.ac.in
URL: http://www.iiserpune.ac.in/~vg.anand/

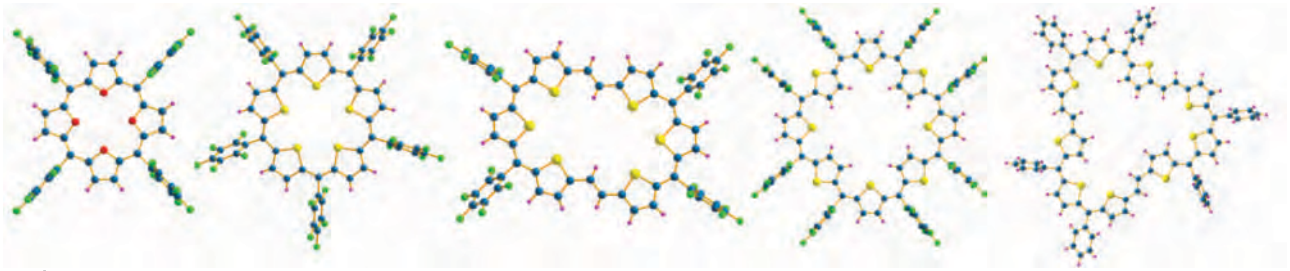
Antiaromaticity

The main research focus of this laboratory is in the design, synthesis and exploration of electronic properties of 4nπ macrocycles derived from small heterocycles such as thiophene, furan, and selenophene.



Huckel's rule suggests a reversible two-electron redox reaction between aromatic and antiaromatic states for planar π-conjugated macrocycle. However, such observations are very rare and limited to smaller hydrocarbon rings. In pursuit of stable 4nπ systems, we have synthesized a range of 4nπ-expanded isophlorins bearing 20π to 48π electrons. The structure of isophlorin was hypothesized as a possible unstable intermediate in the synthesis of porphyrin. We were successful in the synthesis of the first stable 20π isophlorins derived from furan and thiophene heterocycles. Spectroscopic characterization and structural elucidation confirmed its antiaromatic nature in solution and solid states. In continuation with this study, we were successful in the isolation and characterization of an air-stable neutral 25π penta-thiophene macrocycle. It undergoes one-electron redox reactions to form 26π aromatic anion and 24π antiaromatic cation. All the three states of this rare organic redox states were characterized in solution and solid state. Much larger antiaromatic expanded isophlorins with 32π electrons exhibited reversible two-electrons oxidation to 30π aromatic dication. The larger macrocycles bearing 40π and 48π electrons were also found to be planar and antiaromatic in nature. But their redox properties were found to be different compared to the smaller macrocycles. Our observations reveal significant difference in the redox properties of antiaromatic macrocycles compared to aromatic macrocycles.





Publications

Total number of publications: 31**; Independent publications:** 08

Selected Publications

- Gopalakrishna, T. Y.; Reddy, J. S.; **Anand, V. G**. An Amphoteric Switch to Aromatic and Antiaromatic States of a Neutral Air-Stable 25π Radical. *Angew. Chem. Int. Ed.*, **2014**, *53*, 10984-10987.
- Gopalakrishna, T. Y.; **Anand, V. G.** Reversible Redox Reaction Between Antiaromatic and Aromatic States of 32πExpanded Isophlorins. *Angew. Chem. Int. Ed.*, **2014**, *53*, 6678-6682.
- Gadekar, S. C.; Reddy, B. K.; **Anand, V. G.** Metal Assisted Cyclomerization of N-confused Dipyrrins into Expanded Norroles. *Angew. Chem. Int. Ed.*, **2013**, *52*, 7164-7167.
- Gopalakrishna, T. Y.; Reddy, J. S.; **Anand, V. G.** Antiaromatic Supramolecules: F···S, F···Se, and F···π Intermolecular Interactions in 32π Expanded Isophlorins. *Angew. Chem. Int. Ed.*, **2013**, *52*, 1763-1767.
- Reddy, J. S.; **Anand, V. G.** Aromatic Expanded Isophlorins: Stable 30π Annulene Analogues with Diverse Structural Features. *J. Am. Chem. Soc.*, **2009**, *131*, 15433-15439.

External Grants

- Design, Syntheses and Characterization Modified Dipyrrins and its complexes. Funding Agency: SERB-DST, India (September 2013- August 2016).
- Porphyrin, chlorin and isophlorin based near-infrared dyes for high-efficiency dye-sensitized solar cells: an inspiration from the nature. Funding Agency: India (DST) – Singapore (A*STAR) collaborative project (November 2014- September 2017).

Teaching Contributions

General Chemistry, Introductory Inorganic Chemistry, Main Group Chemistry, Transition Metal Chemistry, Advanced Inorganic Laboratory, All Lab courses and Bioinorganic Chemistry

Awards and Recognitions

- Swarnajaynathi Fellow, Department of Science and Technology, New Delhi, India, 2013.
- Young Scientist Medal, Indian National Science Academy, New Delhi, India, 2009.
- Young Associate, Indian Academy of Sciences, Bengaluru, India, 2008.

Research Group

Post-Doctoral Researchers: Dr. Neelam Shivran

Doctoral students: T. Y. Gopalakrishna, Santosh Gadekar, Kiran Reddy, Santosh Panchal, Rakesh Gaur, Ashok Kumar, Madan Ambhore

Under-graduate students: Manish Kumar

Past doctoral students: Dr. Sreedhar Reddy

Past under-graduate students: Prakhar Arora, Rakesh Gaur and Rajkumar Yadav

NIRMALYA BALLAV

Assistant Professor

Ph.D.: University of Calcutta, Kolkata, India
Post-doc.: University of Heidelberg, Heidelberg, Germany
Post-doc.: Paul Scherrer Institute (ETH Domain), Villigen, Switzerland
Joining at IISER: April 2011
Email: nballav@iiserpune.ac.in
URL: http://www.iiserpune.ac.in/~nballav/

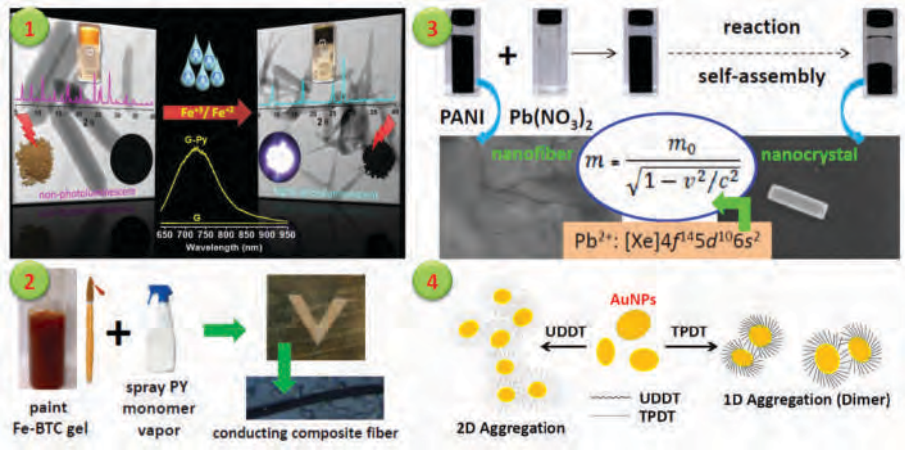
Surface Science and Materials Chemistry

The main research focus of this laboratory is on Surface Science. Until successful establishment of the planned Surface Science Laboratory @ IISER Pune, we are investigating metal, alloy and oxide nanoparticles; metal-organic coordination polymer gels and hybrids; self-assembled nanostructures of conducting polymers and hybrids; and graphene-based materials. We are interested in exploring the broad research area of Materials Chemistry in general.

Redox-active metal-organic gels (MOGs) are evolving as a new class of stimuli responsive materials. MOG comprised of Fe^{3+} ions and benzene tricarboxylic acid (BTC) ligand is prepared and characterized. *In situ* incorporation (without the use of any extraneous oxidant) of conducting polypyrrole and polythiophene moieties into the xerogel matrix was achieved and thereby resulted in the formation of hybrid conductive composite materials. Furthermore, in the presence of small reactive organic molecules like pyrrole, aniline, and bithiophene, the gelation process was unaffected and at the same time it led to the formation of highly photoluminescent hybrid materials (Figure 1 and Figure 2).

Toxic Pb^{2+} ions from aqueous solution could be efficiently removed at ambient conditions with the help of polyaniline (PANI). A significant morphological transformation of PANI from nano-fibers to nano-cuboids suggested a spontaneous and hierarchical self-assembly with Pb^{2+} ions (Figure 3).

Self-assembly of Au nanoparticles in presence of aliphatic dithiol and aromatic dithiol of similar molecular length was found to be remarkably different. Aromatic dithiol lead to the predominant formation of dimers/trimers while aliphatic dithiol induced larger aggregates (Figure 4).



Publications

Total number of publications: 80**; Independent publications:** 27

Selected Publications

- Dhara, B.; Patra, P. P.; Jha, P. K.; Jadhav, S. V.; Pavan Kumar, G. V.; **Ballav, N**. Redox-induced photoluminescence of metalorganic coordination polymer gel. *J. Phys. Chem. C* **2014**, *118,* 19287-93.
- Jha, P. K.; Dhara, B.; **Ballav, N**. Nanofibers to nanocuboids of polyaniline by lead nitrate: hierarchical self-assembly with lead ions. *RSC Adv.* **2014**, *4,* 9851-55.
- Rajendra, R.; **Ballav, N**. Discriminative response of aliphatic and aromatic dithiol in the self-assembly of gold nanoparticles. *RSC Adv. 2013, 3,* 15622-25.
- Dhara, B.; **Ballav, N**. In situ generation of conducting polymer in a redox-active metalorganic gel. *RSC Adv. 2013, 3,* 4909-13.
- Koninti, R. K.; Sengupta, A.; Gavvala, K.; **Ballav, N**.; Hazra, P. Loading of an anti-cancer drug onto graphene oxide and subsequent release to DNA/RNA: a direct optical detection. *Nanoscale* **2014**, *6*, 2937-44.

External Grants

- PI: Two-Dimensional Metal-Organic Coordination Networks. Funding Agency: DAE-BRNS, India. (Feb 2012-Jan 2015).
- Co-PI: Centre for Research in Energy and Sustainable Materials (CORESUM) at IISER-Pune. Funding Agency: MHRD, India. (2014- 2019).
- Co-PI: Chimeric Nanoparticle for Targeting Signalling Network as Next-Generation Cancer Therapeutics. Agency: DBT, India. (2015- 2019).

Teaching Contributions

Advanced Materials Science, Transition Metals Chemistry, Self-Assembly, Inorganic Chemistry, Chemistry Lab I and II (Physical and Inorganic Chemistry), Chemistry Lab II-Inorganic Chemistry, Advanced Inorganic Chemistry Laboratory, Advanced Physical Chemistry Laboratory

Awards and Recognitions

• Sir P. C. Ray Research Award 2003 • Gerhard Ertl Young Investigator Award 2011 • DAE-Young Scientist Research Award 2011 • ChemComm Emerging Investigator 2014 • Visiting Scientist, PSI, Switzerland, 2011- till date

Research Group

Doctoral students: Barun Dhara, Ranguwar Rajendra, Plawan Jha, Shammi Rana

Under-graduate students: Anita Justin

Women scientist: Dr. Sweta Naik

Past under-graduate students: Vimlesh K. Bind, Hetal Vaishnav, Shraddha Jadhav, Shrikant Shende

SUDIPTA BASU

Ramalingaswami Fellow

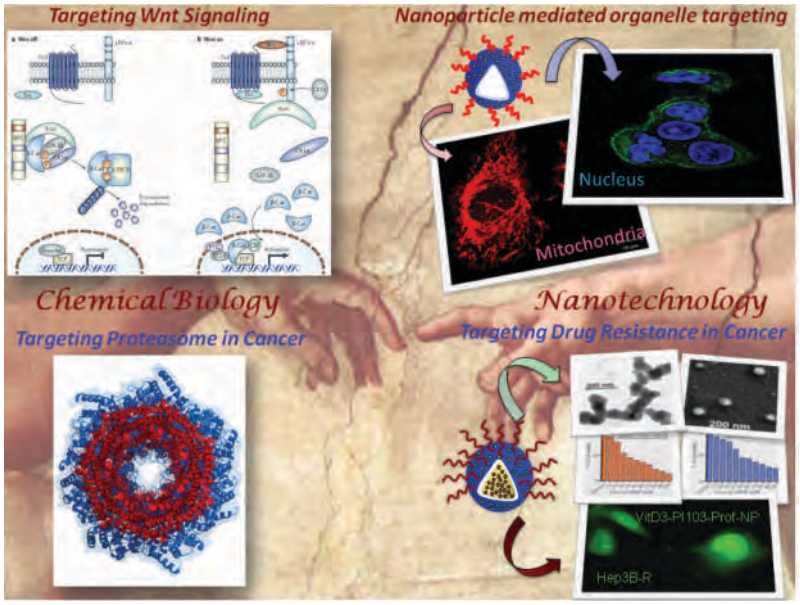
Ph.D.: Max-Planck Institute for Molecular Physiology, Dortmund, Germany
Post-doc.: Brigham and Women's Hospital, Harvard Medical School, Boston, USA
Joining at IISER: February 2012
Email: sudipta.basu@iiserpune.ac.in
URL: http://www.iiserpune.ac.in/~sudipta.basu/

Chemical Biology, Nanotechnology, Signaling in Cancer

The main research focus of this laboratory is to merge synthetic organic chemistry, chemical biology and nanotechnology based tools and techniques to target multiple organelles and signaling pathways in cancer.

Nanotechnology Tools: We have developed biocompatible and biodegradable nanoparticles based on lithocholic acid and vitamin D3 to deliver cytotoxic drugs as well as kinase inhibitors into the cancer cells. We used vitamin D3 nanoparticles to deliver dual drug combination to overcome drug resistance in hepatocellular carcinoma. We engineered nanoparticles from dual drug conjugate to target mitochondria and nucleus simultaneously into cancer cells which could lead to improved efficacy in next generation cancer therapeutics.

Chemical Biology Tools: Wnt signaling has emerged as one of the interesting targets in cancer therapeutics, regenerative medicine, embryonic development and stem cell biology. We are interested to develop novel small molecule library to modulate Wnt signaling in cancer and developmental processes. In recent years proteasome has also emerged as another interesting target for cancer therapeutics considering its role in protein degradation, endoplasmic reticulum stress response and controlling cellular protein homeostasis. We are currently developing small molecule proteasome inhibitors as novel cancer therapeutic agents by using chemical biology tool box.



Publications

Total number of publications: 19**; Independent publications:** 3

Selected Publications

- Patil, S.; Patil, S.; Gawali, S.; Shende, S.; Jadhav, S.; **Basu, S.** Novel Self-Assembled Lithocholic Acid Nanoparticles for Drug Delivery in Cancer. *RSC Adv.* **2013***, 3,* 19760-19764.
- Patil, S.; **Gawali**, S.; **Patil**, S.; **Basu, S.** Synthesis, characterization and in vitro evaluation of novel vitamin D3 nanoparticles as versatile platform for drug delivery in cancer. *J. Mater. Chem. B*, **2013**, *1*, 5742-5750.
- Palvai, S.; Nagraj, J.; Mapara, N.; Chowdhury, R.; **Basu, S.** Dual drug loaded vitamin D3 nanoparticle to target drug resistance in cancer. *RSC Adv.* **2014**, *4*, 57271-57281.

External Grants

- Chimeric Nanoparticle: A Novel Nanoplatform for Signaling Pathway Driven Cancer Chemotherapy. Funding Agency: Ramalingaswami Fellowship, DBT, India (Feb 2012-Jan 2017).
- Engineering Novel Supramolecular Nanoplatform for Paclitaxel Delivery in Cancer. Funding Agency: DST-SERB, India (Aug. 2013-July 2016).
- Chimeric Nanoparticle for Targeting Signalling Network as Next-Generation Cancer Therapeutics, Funding Agency: DBT, India (Dec. 2014-Nov. 2017).

Teaching Contributions

Organic Synthesis II, Bioorganic Chemistry

Awards and Recognitions

- Ramalingaswami Fellowship (DBT, India)
- Charles A. King Trust Post-doctoral Research Fellowship Award (USA)

Research Group

Doctoral and project students: Abhik Mallick, Sandeep Palvai, Chandramouli Ghosh, Sohan Patil, Aditi Dixit, Piyush More, Nikunj Mapara.

Under-graduate students: Syed Muhammed Muazzam Kamil.

Past under-graduate students: Suhas Gawali, Sumersing Patil, Deepali Kothurkar, GKRS Naresh

RAMAKRISHNA G. BHAT

Associate Professor

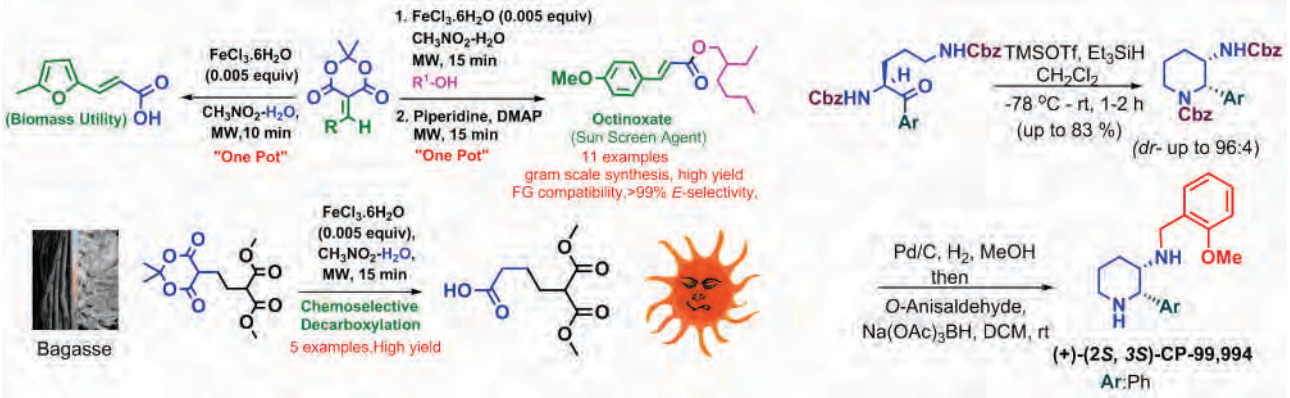
Ph.D.: Indian Institute of Science, Bangalore, India
Post-doc.: Simon Fraser University, British Columbia, Vancouver, Canada
Visiting Faculty: July 2006 –April 2007, IISER-Pune
Assistant Professor: May 2007 –January 2013, IISER-Pune
Associate Professor: January 2013 – Present date, IISER-Pune
Email: rgb@iiserpune.ac.in
URL: http://www.iiserpune.ac.in/~rgb/

Organic Synthesis, Catalysis and Medicinal Chemistry

The main research focus of our laboratory is in the field of organic synthesis with a focus on green asymmetric catalytic synthesis and C-H/C-X bond functionalization. Emphasis is on the development of new synthetic methods that facilitate the construction of complex and bioactive molecules. Some of the strategies developed will be employed for the enantioselective synthesis of bioactive natural products and also for the synthesis inhibitors of PI-3 and aurora kinases.

An easy access to *a, β*-unsaturated carboxylic acids and esters and *cis*-2, 3-disubstituted piperidines:

We developed a novel, practical and convenient catalytic protocol comprising of $FeCl_3.6H_2O$-CH_3NO_2-H_2O for the rapid synthesis of *a, β*-unsaturated carboxylic acids and esters with high *E*-stereoselectivity both under microwave and conventional heating conditions. This powerful approach efficiently demonstrated the utility of biomass derived aldehydes to make fuel additives. One pot route to cinnamate esters has been explored by the synthesis of commercial sunscreen agents. This protocol has been proved to be a general method for the gram scale synthesis.



(*a, β*-Unsaturated carboxylic acids and esters) (Novel approach to *cis*-2,3-disubstituted piperidines)

We have developed an efficient and useful approach for constructing *cis*-2-aryl 3-amino piperidines with an option of introducing diverse aryl groups at C-2 position. This also gives an easy access to condense different aldehydes at C-3 amine functionality without compromising the stereochemistry. Application of this method has been exemplified in the enantioselective sythesis of (+)-CP-99,99, NK1-receptor antagonist. Currently we are focusing our efforts on asymmetric intermolecular C-H functionalization using nontoxic metal catalysts at ambient conditions and asymmetic catalysis.

Publications

Total number of publications: 18 **; Independent publications:** 8, **Patent:** 1 applied

Selected Publications

- Sultane, P. R.; Mete, T. B.; **Bhat, R. G**. Chemoselective N-deacetylation under mild conditions *Org. Biomol. Chem*. **2014**, *12*, 261-264. (Highlighted in *ChemInform*, 2012, 43, Issue 17)
- Mohite, A. R.; **Bhat, R. G**. A Practical and Convenient Protocol for the Synthesis of (E)-α,β-Unsaturated Acids *Org. Lett.* **2013**, *15*, 4564-4567. (Highlighted in *Organic Chemistry Portal*)
- Sultane, P. R.; **Bhat, R. G**. Stereoselective Approach to cis-2,3-Disubstituted Piperidines via Reduction of N-Acyliminium Ion Intermediate: Enantioselective Synthesis of (+)-(2S,3S)-CP-99,994 *J. Org. Chem.* **2012**, *77*, 11349-11354. (Highlighted in *Organic Chemistry Portal*)
- Mohite, A. R. and **Bhat, R. G.** Enantiopure Synthesis of Side Chain-Modified α-Amino Acids and 5-cis-Alkylprolines. *J. Org. Chem*. **2012**, *77*, 5423–5428.
- Mohite, A. R., Sultane, P. R., and **Bhat, R. G.** $BF_3.Et_2O$ and Trifluoroacetic acid/Triethyl amine mediated synthesis of Functionalized Piperidines. *Tetrahedron Lett.* **2012**, *53*, 30-35. (Highlighted in *ChemInform*, 2012, 43, Issue 17)

Teaching Contributions

Introductory General Chemistry-Freshman Course (Organic Chemistry), Chemistry of Elements, Chemistry II-(Organic Chemistry), Organic Synthesis-I -Advanced Course, CHM411-Organic Synthesis-II, Medicinal Chemistry, Chemistry Practical (Organic chemistry Practicals), Advanced Organic Chemistry Practical

Research Group

Doctoral and project students: L. V. S. Rajesh Babu, Balu S. Navale, Tushar M. Khopade, Trimbak B. Mete, Rameshwar Shinde

Under-graduate students: Abhishek Soni

Past doctoral students: Dr. Amar R. Mohite Dr. Prakash R. Sultane

Past under-graduate students: Digvijay Porwal, Shishir Chourey

R. BOOMI SHANKAR

Associate Professor

Ph.D.: Indian Institute of Technology, Kanpur, India
Post-doc.: University of Illinois, Urbana-Champaign, USA
Post-doc.: University of Liverpool, UK
Assistant Professor: April 2008 – December 2010, IIT-Guwahati
Assistant Professor: December 2010 – December 2014, IISER-Pune
Associate Professor: December 2014 – Present date, IISER-Pune
Email: boomi@iiserpune.ac.in
URL: http://www.iiserpune.ac.in/~boomi/

Main Group, Organometallic and Materials Chemistry

The main research focus of the group is on developing novel molecular systems derived from the elements of group 13, 14 and 15 and their applications in materials chemistry and catalysis. Significant strides have been made by employing organosilicon and amino-P(V) scaffolds containing central as well as peripheral metal binding groups.

Facile routes to access P(V)-imido anions in polar and in protic solvents have been developed by employing the salts certain reactive soft metal ions, such as Ag(I), Cu(I) and Pd(II) ions. Novel examples of tri- and hexanuclear Pd(II) complexes stabilized by the highly basic tris(imido)- phosphate trianions were reported for the first time. Further, these complexes were used as supramolecular synthons for obtaining elusive neutral polyhedral cages for Pd(II) ions and their host-guest behaviour was studied extensively (Figure 1). Apart from these, several peripherally functionalized imido and amido-P(V) ligands have been explored for their functional properties viz. selective gas and solvent uptake studies, guest-induced physical properties etc.

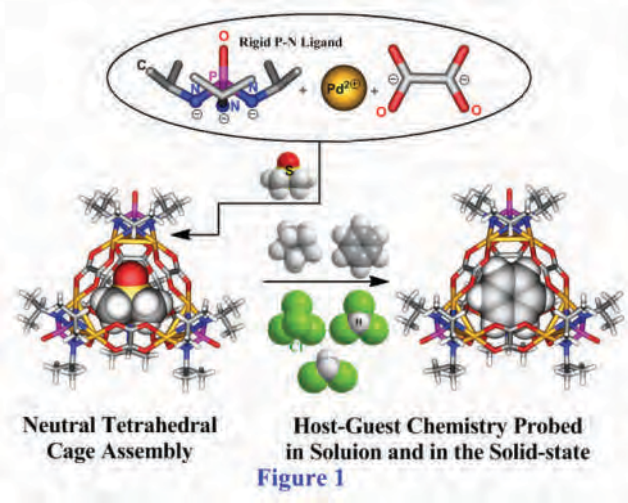


Figure 1

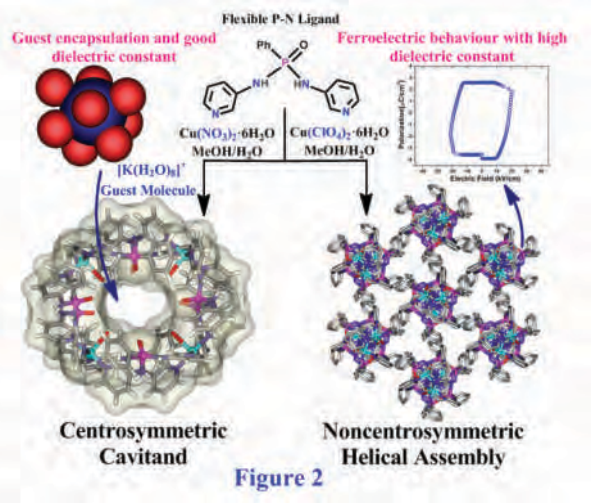


Figure 2

Organic and metal-organic ferroelectric materials have been prepared from main group moieties containing appropriate symmetry. Noticeably, tunable ferroelectric behaviour with high saturation polarization values and high dielectric constant values have been achieved for various examples of anion driven $Cu^{II}L_2$ frameworks (Figure 2).

Photo-functional cluster MOFs of unusual copper (I) iodide clusters have been synthesized using tripodal phosphoramide or organosilane platforms. These cluster MOFs were shown to exhibit stimuli-responsive luminescence behaviour such as thermochromism and mechanochromism.

Publications

Total number of publications: 42**; Independent publications:** 15

Selected Publications

- Srivastava, A. K.; Praveen Kumar, B.; Mahawar, I. K.; Divya, P.; Shalini, S.; **Boomishankar, R.** Anion Driven $[Cu^{II}L_2]_n$ Frameworks: Crystal Structures, Guest-Encapsulation, Dielectric, and Possible Ferroelectric Properties. *Chem. Mater.* **2014**, *26,* 3811-3817.
- Yadav, A.; Srivastava, A. K.; Balamurugan, A.; **Boomishankar, R.** A Cationic copper(I) iodide cluster MOF exhibiting unusual ligand assisted thermochromism. *Dalton Trans.* **2014**, *43,* 8166-8169.
- Gupta, A. K.; Reddy S. A. D.; **Boomishankar, R.** Facile formation of stable tris(imido)phosphate trianions as its tri- and hexa-nuclear Pd(II) complexes in polar solvents. *Inorg. Chem.* **2013**, *52*, 7608-7614.
- Gupta, A. K.; Nagarkar S. S.; **Boomishankar, R.** Zn(II) coordination polymer of an in-situ generated 4-pyridyl (^{4}Py) attached bis(amido)phosphate ligand, $[PO_2(NH^4Py)_2]^-$ showing preferential water uptake over aliphatic alcohols. *Dalton Trans.* **2013**, *42*, 10964-10970.
- Gupta, A. K.; Chipem F. A. S.; **Boomishankar, R.** A 2-pyridyl (py) attached phosphine imine $[P(Npy)(NHpy)_3]$ and an imido phosphinate ion $[P(Npy)_2(NHpy)_2]^-$ in its Ag(I) complex. *Dalton Trans.* **2012**, *41*, 1848-1853.

External Grants

- Peripherally functionalized siloxane scaffolds for the assembly of multi-metallic cages, cluster and supramolecules. Funding Agency: SERB-DST, India (May 2013-April 2016).
- Design and synthesis of functional framework materials based on P-N and P-O building blocks. Funding Agency: SERB-DST, India (March 2009- September 2012).

Teaching Contributions

Introductory Inorganic Chemistry, Chemistry Lab II-Inorganic Chemistry, Main Group Chemistry, Advanced Inorganic Chemistry, Advanced Inorganic Laboratory

Research Group

Doctoral and project students: Anant Kumar Srivastava, Mahesh Deshmukh, Ashok Yadav, P. Rajasekar, T. Vijaikanth, Sheik Sadam Husein

Under-graduate students: Sourabh

Past doctoral students: Dr. Arvind Gupta

Past under-graduate students: Arun Dixith Reddy, Indra Mahawar

B. GNANAPRAKASAM

Assistant Professor

Ph.D.: Central Salt and Marine Chemicals Research Institute, Bhavnagar
Post-doc: University of Goettingen, Goettingen, Germany
Post-doc: Weizmann Institute of Sciences, Rehovot, Israel
Previous position: Scientist, ICES, A*STAR, Singapore:
Associate Professor, SRM Research Institute, Chennai
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Natural Products Synthesis and Homogeneous Catalysis

The main research focus of the laboratory is to develop efficient and novel sustainable route to synthesize natural products of challenging structures with intriguing biological activities. Towards this, new catalytic reactions for stereoselective domino reactions, phenolic oxidation and dehydrogenate coupling reactions will be attempted using cooperative metal catalysts that eventually lead to stereoselective C-C, C-N and C-O bonds formation. Various key building blocks can be synthesized by avoiding hazardous stoichiometry reagents and activators utilizing these protocols.

Asymmetric synthesis: Our research focus is to develop sustainable and efficient methods for the synthesis of chiral amines and related analogues which are widely used in chemical industry via enantioselective amination using alcohols, alkenes or alkynes and chiral cooperative metal catalyst.

Flow mediated organic transformations: Considering the potential application of flow chemistry in the pharmaceutical industry and fine chemicals synthesis, basic research is desirable in implementing the batch processes into flow chemistry for challenging organic transformations. We are interested in developing a new process for the conversion of easily available alcohols or esters into respective dehydrogenated products using metal catalyst under continuous flow techniques.

Fluorination methods: Our research aim is to study the catalytic fluorination of various activated/un-activated aromatic and non-aromatic compounds using cooperative metal complex catalyst, non-hazardous and inexpensive fluorinating agents.

Publications

Total number of publications: 18**; Patents:** 2

Selected Publications

- Tietze, L. F.; Ma, L.; Jackenkroll, S.; Reiner, J. R.; Hierold, J.; **Gnanaprakasam, B.** and Heidemann, S. The paecilin puzzle. Enantioselective synthesis of the proposed structures of paecilin A and B. *Heterocycles*, **2014**, *88*, 1101-1119.

- **Gnanaprakasam, B.**; Balaraman, E.; Ben-David, Y and Milstein, D. Synthesis of peptides and pyrazines from amino alcohols through extrusion of H_2 catalyzed by Ruthenium pincer complexes: Ligand-controlled selectivity. *Angew. Chem.*, **2011**, *50*, 12240-12244.
- **Gnanaprakasam, B.** and Milstein, D. Direct synthesis of amides from esters with liberation of H_2 under Neutral Conditions. *J. Am. Chem. Soc.* **2011**, *133*, 1682.
- **Gnanaprakasam, B.**; Zhang, J and Milstein, D. Direct synthesis of imines from alcohols and amines with liberation of H_2. *Angew. Chem.* **2010**, *49*, 1468-1471.
- **Gnanaprakasam, B.**; Ben-David, Y and Milstein, D. Ruthenium-pincer catalyzed acylation of alcohols using esters with liberation of H_2 under neutral conditions. *Adv. Synth. Cat.* **2010**, *352*, 3169-3173.

External Grants

- Studies on Metal Catalyzed Stereoselective C-C, C-N and C-O Bond Formation via Borrowing Hydrogen Methods Using Continuous Flow Techniques. Funding Agency: SERB-DST, India. (Submitted)

Teaching Contributions

Organic Photochemistry, Chemistry Laboratory III

Awards and Recognitions

- Alexander Von Humboldt Fellow (2012)

Research Group

Project student: Moreshwar B Chaudhari

HARINATH CHAKRAPANI

Assistant Professor

Ph.D.: Duke University, North Carolina, USA
Post-doc.: Wake Forest University, North Carolina, USA
Post-doc.: National Cancer Institute, Maryland, USA
Joining at IISER: July 2009
Email: harinath@iiserpune.ac.in
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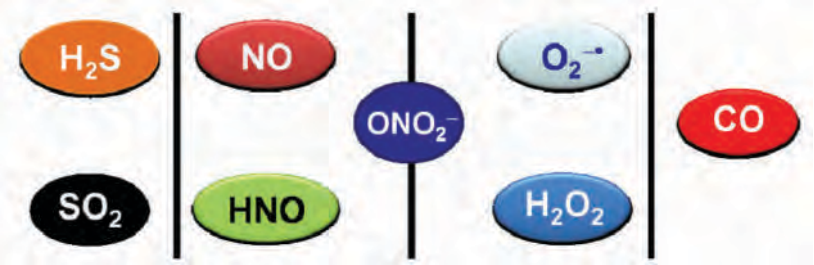
Organic Chemistry and Chemical Biology

The main research focus of our lab is the development of small organic molecules for controlled generation and release of short-lived biological species such as reactive nitrogen, oxygen and sulfur species. In order to achieve controlled release, we design and develop small molecule based probes. These small molecules can be used as tools for studying the chemistry and biology of such reactive species and might also allow us to explore the potential for therapeutic applications as well.



Reactive oxygen species (ROS) are produced inadvertently in nearly all organisms. Superoxide O_2, which is produced by 1-electron transfer to oxygen during respiration and is subsequently converted to hydrogen peroxide H_2O_2, which through the Fenton reaction generates the highly reactive OH. Together, these ROS can damage vital cellular components and are hence deployed by the immune system to counter infectious pathogens. Several recent studies have shown that ROS can sensitize infectious bacteria to clinical antibiotics suggesting the possible therapeutic utility for ROS. Our goal is to design and develop small molecule generators of ROS in order to better understand cellular responses to elevated ROS.

Reactive sulfur species are produced as intermediates during sulfur metabolism. Hydrogen sulfide (H_2S) is generated but precise mechanisms of its actions are not known. During oxidative conditions, H_2S is converted to sulfur dioxide (SO_2), which primarily exists as its hydrated from, sulfite. This reactive sulfur species is used in wine making as an antibacterial and the food industry as a preservative and antioxidant. We have developed several small molecules that can produce reactive sulfur species in a controlled manner and demonstrated their antibacterial properties.

Nitric oxide (NO) is a versatile biomolecule that mediates numerous physiological processes. The therapeutic potential of NO has been recognized but few promising methodologies for the use of NO as are available. This is attributable primarily to the toxicity associated with elevated levels of NO. For example, numerous studies demonstrate the efficacy of NO as a potent tumoristatic agent. However, due to its

multifarious biological effects, controlled and localized generation of therapeutic NO using prodrugs is necessary. Other studies have shown antimicrobial effects of NO especially against drug resistant bacteria. We developed several small molecule strategies for localizing and monitoring nitric oxide within cells.

Publications

Total number of publications: 42**; Independent publications:** 15

Selected Publications

- Sankar, R. K; Kumbhare, R. S.; Dharmaraja, A. T.; **Chakrapani, H.** A Phenacrylate Scaffold for Tunable Thiol Activation and Release. *Chem. Commun.* **2014**, *50*, 15323-15326.
- Dharamaraja, A. T; **Chakrapani, H.** A Small Molecule for Controlled Generation of Reactive Oxygen Species (ROS) *Org. Lett.*, **2014**, *16*, 398-401.
- Khodade, V. S.; Sharath Chandra, M.; Banerjee, A.; Lahiri, S.; Pulipeta, M.; Rangarajan, R.; **Chakrapani, H**. Bioreductively Activated Reactive Oxygen Species (ROS) Generators as MRSA Inhibitors. *ACS Med. Chem. Lett.* **2014**, *5*, 777-781.
- Sharma, K.; Iyer, A.; Sengupta, K.; **Chakrapani, H**. INDQ/NO, a Bioreductively Activated Nitric Oxide Prodrug. *Org. Lett.*, **2013**, *15*, 2636–2639.
- Malwal, S. R.; Sriram, D.; Yogeeswari, P.; Konkimalla, V. B.; **Chakrapani, H**. Design, Synthesis and Evaluation of Thiol-Activated Sources of Sulfur Dioxide (SO_2) as Antimycobacterial Agents. *J. Med. Chem.*, **2012**, *55*, 553-557.

External Grants

- Hypoxia-Activated Prodrugs of Nitric Oxide. Funding Agency: DBT, India (Mar 2012-Mar 2015).
- Redox-Directed Mycobacterial Therapeutics. Funding Agency: DBT, India (Nov 2012- Sep 2015).

Teaching Contributions

Introductory Organic Chemistry, Chemistry Lab III-Organic Chemistry, Physical Organic Chemistry, Medicinal Chemistry, Advanced Organic Laboratory, Organic Synthesis I, Organic Synthesis II and Practice of Science: Ethics, Safety and Communication

Awards and Recognitions

- Innovative Young Biotechnologist Award, 2011
- Early Career Scientist, 2012; Royal Society of Chemistry-West India

Research Group

Doctoral and project students: Satish Malwal, A. Dharmaraja, Kavita Sharma, Vinayak Khodade, Kundansingh Pardeshi, G. Ravikumar, Amogh Kulkarni, Preeti Chauhan, Ajaykumar Sharma, R. K. Sankar, and Viraj Gala

Under-graduate students: M. Sharathchandra

Past under-graduate students: Rohan Kumbhare

SRABANTI CHAUDHURY

Assistant Professor

Ph.D.: Indian Institute of Science, Bangalore, India
Post-doc.: Rice University, Houston, USA
Post-doc.: University of Texas at Austin, Austin, USA
Post-doc.: Los Alamos National Laboratory, USA
Joining at IISER: April 2013
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Theoretical Biophysical Chemistry

The main research focus of my group is on developing analytical models based on the principles of time dependent statistical mechanics and applying them to investigate problems in chemical physics, biological physics and soft condensed matter. Our analytical findings are properly complemented with simulations and available experimental results.

Modeling the effect of transcriptional noise on switching in gene networks in a genetic bistable switch: A new theoretical method has been proposed to study the dynamics of switching in a two state gene expression model by explicitly accounting for the transcriptional noise. This theoretical technique along with Monte Carlo simulations has been used to study how switching times starting from either active/inactive promoter state are affected by different biological parameters such as transcription rate and so on.

Modeling the effect of allosteric inhibition in single molecule enzyme kinetics: In this project we are studying the turnover statistics of a single enzyme in the presence of inhibitors for different types of enzyme inhibitor reactions. We have developed a theoretical formalism to calculate the effect of temporal fluctuations in the reaction rate in the presence of inhibitors as observed at the single molecule level. Our theory has been used to study enzymatic inhibition kinetics in a single molecule experiment where individual enzyme molecules inhibited by the product.

Publications

Total number of publications: 16 **; Independent publications:** 1

Selected Publications

- **S. Chaudhury**, Poison indicator and Fano factor in probing dynamic disorder in single molecule enzyme inhibition kinetics. *J. Phys. Chem. B* **2014**, *118*, 10405.
- **S. Chaudhury**, N. A. Sinitsyn and A. S. Perelson, Spontaneous clearance of viral infections by mesoscopic fluctuations. *PLoS ONE* **2012**, e38549.

- **S. Chaudhury** and D. A. Makarov, A harmonic state approximation for the duration of reactive events in complex molecular rearrangements. *J. Chem. Phys.* **2010**, *133*, 034118.
- **S. Chaudhury** and B. J. Cherayil, A model of anomalous chain translocation dynamics. *J. Phys. Chem. B* **2008**, *112*, 15973.
- **S. Chaudhury** and B. J. Cherayil, Complex chemical kinetics in single enzyme molecules: Kramers model with fractional Gaussian noise. *J. Chem. Phys.* **2006**, *125,* 024904.

External Grants

- Modelling heterogeneity in nanoparticle catalysis at the single molecule level, Start-Up Research Grant (Young Scientists) Funding Agency: SERB-DST, India (approved).

Teaching Contributions

Symmetry and Group Theory, Statistical Thermodynamics

Research Group

Doctoral and project students: Bappa Ghosh

Past project students: Anusheela Das

JEETENDER CHUGH

Assistant Professor

Ph.D.: Tata Institute of Fundamental Research, Mumbai, India
Post-doc.: University of Michigan, Ann Arbor, USA
Joining at IISER: March 2014
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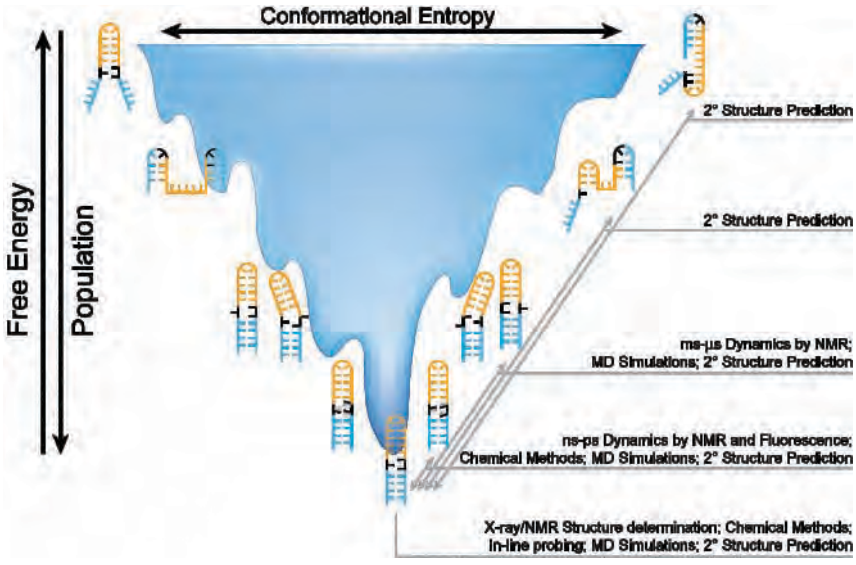
URL: http://www.iiserpune.ac.in/~cjeet/

NMR Spectroscopy of Biomolecules

The main research focus of my laboratory is on theoretical design and experimental implementation of new NMR experiments to probe the biophysical characteristics of RNA and proteins; understanding functional aspects of non-coding RNAs; and structural biology of microRNAs and their regulation in various disease settings.

Developing sequence codes for ms-μs dynamics in RNA With the current plethora of structure prediction algorithms, it is possible to predict sub-optimal secondary structures for a given RNA sequence. However, the number of these sub-optimal secondary structures, as predicted by various structure prediction algorithms available, increases exponentially both with increase in the number of nucleotides in the RNA sequence and with increase in the energy range. Although, for small RNAs and for small energy range these algorithms do pretty well, but still there is a need to validate these 'feasible' structures experimentally. Experimental characterization of alternative structures for small RNAs using state-of-the-art $R_{1\rho}$ NMR relaxation dispersion experiments has been done successfully but is a time consuming and expensive affair. Thus there is a dire need to formulate sequence codes that would predispose the sequence towards such motions and allow predicting precise sub-optimal secondary structures without the need of experiments.



Expanding current structural understandings of miRNA biogenesis pathway All miRNAs do not follow a universal pathway for their biogenesis. Specific mechanisms in the biogenesis of individual class of miRNAs suggest multiple opportunities for tight regulation of miRNA levels. This spectrum of distinct mechanisms is widening everyday as more and more interacting partners are being identified. Although several reports emphasize on the regulatory activities of miRNAs, very little is known about the structural (primary, secondary or tertiary) understanding of the regulation of miRNA expression levels and their activity. Therefore, understanding the conformational roles fundamental for these regulatory mechanisms in the miRNA biogenesis pathway may act as a path-breaking step for development of new drugs based on RNAi mechanism.

Publications

Total number of publications: 24**; Independent publications:** 1

Selected Publications

- **Chugh, J.** Determining Transient Nucleic Acid Structures by NMR. *Chemical Biology of Nucleic Acids; RNA Technologies*. Springer **2014**, 181-198. (Book Chapter)
- Zeng, X.; **Chugh, J.**; Casiano-Negroni, A.; Al-Hashimi, H. M.; Brooks III, C. L. Flipping of the ribosomal A-site adenines provides a basis for tRNA selection. *J. Mol. Biol.* **2014**, *426(19)*, 3201-3213.
- Dethoff, E. A.*; Petzold K.*; **Chugh, J.***; Casiano-Negroni, A.; Al-Hashimi, H. M. FVisualizing Transient Low-Populated Structures of RNA. *Nature* **2012**, *491(7426)*, 724-728.
- Dethoff, E. A.*; **Chugh, J.***; Mustoe, A. M.; Al-Hashimi, H. M. Functional Complexity and Regulation through RNA Dynamics. *Nature*. **2012**, *482(7385)*, 322-330.
- Bothe, J.; Nikolova E.; Eichhorn, C.; **Chugh, J.**; Hansen, A.; Al-Hashimi, H. M. Charaterizing RNA Dynamics at Atomic Resolution Using Solution-state NMR Spectroscopy. *Nature Methods*. **2011**, 8(11), 919-931.

External Grants

- Applied to DST and Wellcome-DBT Intermediate Fellowship.

Teaching Contributions

Chemistry Laboratory-I Physical Chemistry, Advanced Physical Chemistry Laboratory, Structural Methods and Analysis, Guest Lecturer at University of Pune (Biotechnology Department and Bioinformatics Department)

Research Group

Doctoral students: Himani Rawat, Harshad Paithankar

ALOKE DAS

Associate Professor

Ph.D.: Indian Institute of Technology, Kanpur, India
Post-doc.: Purdue University, USA
Post-doc.: Lawrence Berkeley National Lab and Louisiana State University, USA
Assistant Professor: October 2007 – January 2013, IISER-Pune
Associate Professor: January 2013 – Present date, IISER-Pune
Email: a.das@iiserpune.ac.in
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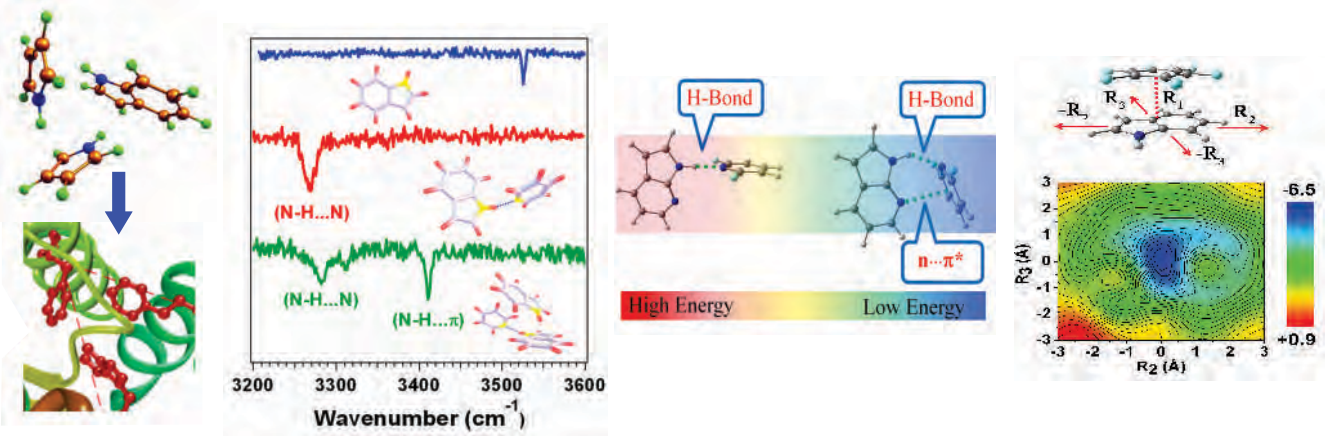
Gas Phase Laser Spectroscopy, Non-covalent Interactions

The main research focus of the group is on molecular level understanding of weak non-covalent interactions responsible for the stabilization of specific structures of biomolecules (proteins, DNA etc.) and materials by using home-built jet-cooled REMPI (Resonantly Enhanced Multiphoton Ionization) Laser-desorption Time of Flight Mass spectrometer.

Competition between electrostatic and dispersion interactions in N-heterocyclic aromatic complexes has been studied in a supersonic jet using R2PI (Resonant two photon ionization), IR-UV and UV-UV double resonance spectroscopic techniques combined with quantum chemistry calculations. Indole has been chosen as central molecular system of study and the complexing partners are pyridine, furan, thiophene, pyrrole, imidazole, and hexafluorobenzene. It has been found that the interactions present in the observed V-shaped, cyclic triangular, tilted T-shaped, and π-stacked complexes resemble with those in biomolecules and materials.



Gas phase spectroscopic evidence of $n \rightarrow \pi^*$ interaction has been explored by studying complexes of 7-azaindole and 2, 6-fluorosubstituted pyridines. The $n \rightarrow \pi^*$ interaction has been probed by measuring the strength of the hydrogen bonding interaction. Direct spectroscopic evidence of the $n \rightarrow \pi^*$ interaction is underway.

Sequence dependent folding motifs of isolated as well as microhydrated peptides are investigated in the gas phase by studying mass selected electronic and vibrational spectroscopy of end-protected tripeptides of different sequences.

Publications

Total number of publications: 31**; Independent publications:** 10

Selected Publications

- Kumar, S.; Singh, S. K.; Calabrese, C.; Maris, A.; Melandri*, S.; **Das, A.*** Structure of saligenin: Microwave, UV and IR spectroscopy studies in a supersonic jet combined with quantum chemistry calculations. *Phys. Chem. Chem. Phys.* **2014**, *16*, 17163-17171.
- Singh, S. K.; Kumar, S.; **Das, A.*** Competition between n→π* and conventional hydrogen bonding (N-H...N) interactions: An ab initio study of the complexes of 7-azaindole and fluorosubstituted pyridines. *Phys. Chem. Chem. Phys.* **2014**, *16*, 8819-8827. (Front inside cover page).
- Kumar, S.; **Das, A.*** Observation of exclusively π-stacked heterodimer of indole and hexafluoro-benzene in the gas phase. *J. Chem. Phys.* **2013**, *139*, 104311.
- Kumar, S.; **Das, A.*** Mimicking trimeric interactions in the aromatic side chains of the proteins: A gas phase study of indole...$(pyrrole)_2$ heterotrimer. *J. Chem. Phys.* **2012**, *136*, 174302. (Selected for Virtual Journal of Biological Physics Research, Vol. 23, May 15, 2012, Section: Protein Conformational Dynamics/Folding)
- Kumar, S.; Pande, V.; **Das, A.*** π-hydrogen bonding wins over conventional hydrogen bonding interaction: A jet-cooled study of indole...furan heterodimer. *J. Phys. Chem. A* **2012**, *116*, 1368-1374.

External Grants

- Conformation of microhydrated peptides: Laser desorption jet-cooled studies. Funding Agency: SERB-DST, India. (March 2012-March 2015).

Teaching Contributions

Introductory Physical Chemistry, Chemistry Lab I-Physical Chemistry, Spectroscopy practicals, Fundamentals of Spectroscopy, Advanced Molecular Spectroscopy

Research Group

Doctoral students: Santosh K. Singh, Neha Sharma, Kamal Kumar Mishra

Under-graduate students: Ajay Kumar

Past doctoral students: Dr. Sumit Kumar

KRISHNA N. GANESH

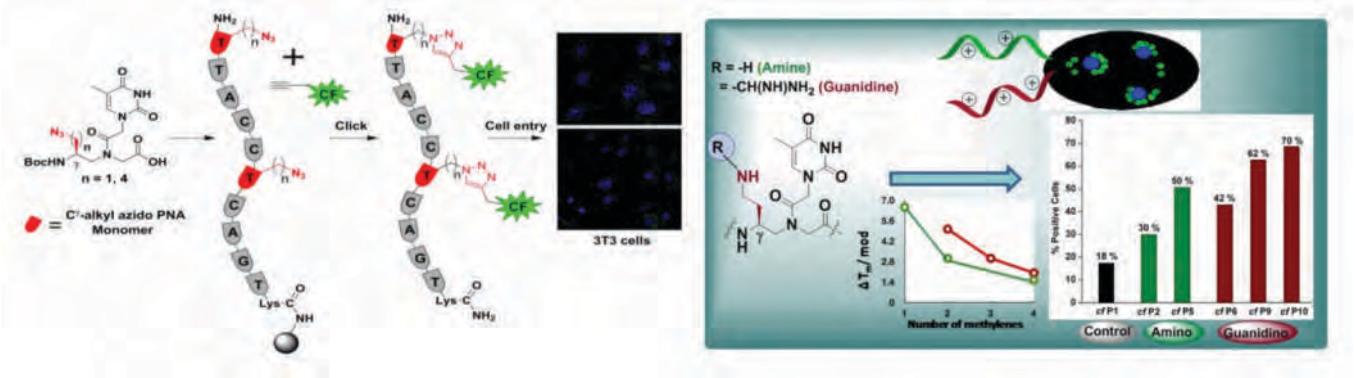
Professor

Ph.D.: University of Delhi, India; Cambridge University, UK
Previous positions: Scientist, Centre for Cellular and Molecular Biology, Hyderabad 1981-1987); Scientist, National Chemical Laboratory, Pune (1987-2006); Professor and Founder Director, IISER Pune (2006 – present).
Joining at IISER: June 2006
Email: kn.ganesh@iiserpune.ac.in
URL: http://www.iiserpune.ac.in/~kn.ganesh/

Biomolecular Chemistry of Peptides and Nucleic Acids

The main research focus of this laboratory is on developing novel Peptide Nucleic acid analogues to enable facile entry into cells and be functional in suppressing the targeted gene expression. These involve inherently cationic PNAs and fluorinated PNAs. We are interested in examining the mechanism of their cell entry, targeting to specific cells and ability to inhibit the expression of target gene. We have specifically demonstrated that the cationic PNAs enter the cells and accumulate around the nuclear membrane region. By conjugation with trimers of N-galactosylamine, these are being now targeted into hepatocyte cells.

Another area of our interest is on studying the cationic 4(*R*/*S*)-substituted collagen mimetic peptides. These form interesting PPII helices, beta structures and show pH and solvent mediated conformational variations. They are also interesting cell penetrating peptides and exhibit unusual self-assembling properties. We are also studying interesting nanostructures of rods and wires formed by assembly of 4(R/S-amino)polyproline peptides and fluoro peptide nucleic acids.



Publications

Total number of publications: 160**; From IISER Pune:** 19

Selected Publications

- Patwa, A. N.; Gupta, S.; Gonnade, R. G.; Kumar, V. A.; Bhadbhade, M. M.; **Ganesh, K. N.**, Ferrocene-Linked Thymine/Uracil Conjugates: Base pairing Directed Self-Assembly and Supramolecular Packing. *J. Org. Chem.* **2008**, *73*, 1508-1515.

- Mahesh V. Sonar and **Krishna N. Ganesh**, Switching structures by H-bond rearrangement: Transformation of β–structure in poly-4*S*-Aminoproline to PPII conformation, *Org. Lett*, **2010**, *12*, 5406-5409.
- Manaswini Nanda and **Krishna N. Ganesh**, 4(*R*/*S*)-Guanidinylprolyl Collagen Peptides: On-resin synthesis, complexation with plasmid DNA, and the role of peptides in enhancement of transfection, *J. Org. Chem*. **2012**, *77*, 4131-4135.
- **Krishna N. Ganesh** and Yamuna Krishnan, Nucleic Acids - Chemistry and Applications. *J. Org. Chem*. **2013**, *78*, 12283 - 12287.
- Deepak Ramesh Jain, Libi Anandi V., Mayurika Lahiri, and **Krishna N. Ganesh**, Influence of pendant chiral Cγ-(alkylideneamino/guanidino) cationic sidechains of PNA backbone on hybridization with complementary DNA/RNA and cell Permeability, *J. Org. Chem*. **2014**, *79*, 9567-9577.

Teaching Contributions

General Chemistry, Bio-organic Chemistry, Chemical Biology, Self-assembly

Awards and Recognitions

- **Fellow**: Indian Academy of Sciences, Bangalore (1995); Indian National Academy of Sciences, New Delhi (1999); National Academy of Sciences, Allahabad (1996); The World Academy of Sciences (TWAS), Trieste (2007)
- **Awards**: SS Bhatnagar Award in Chemical Sciences (1998); TWAS Prize in Chemical Sciences (2006); SASTRA-CNR Rao Award (Chemical Sciences) (2014)
- **President**, Organic and Biomolecular Chemistry Division (Div III), IUPAC (2012-2013)
- **Membership of Editorial Boards of Journal:** International Advisory Board, Journal of Organic Chemistry (ACS, USA); Editorial Advisory Board, Chemistry: Asian Journal (Wiley, Germany); Beilstein Journal of Organic Chemistry (Beilstein Publishing, Germany); Artificial DNA: PNA, XNA (Taylor and Francis, USA); Nature Scientific Reports (NPG, London); Oligonucleotides

Research Group

Doctoral and project students: Nitin Bansode, Vijay Kadam, Satheesh Elelipilli, Madan Gopal, Shahaji More, Prabhakar Pawar, Pramod Bhingardeve, Manoj Kumar Gupta, Pradnya Kulkarni (NCL)

Post-doctoral: Dr. Dhrubajyoti Dutta

Under-graduate students: Pramod Kumar

Past doctoral students: Dr. Deepak Jain, Dr Tanpreet Kaur (NCL); Dr Mahesh Sonar (NCL)

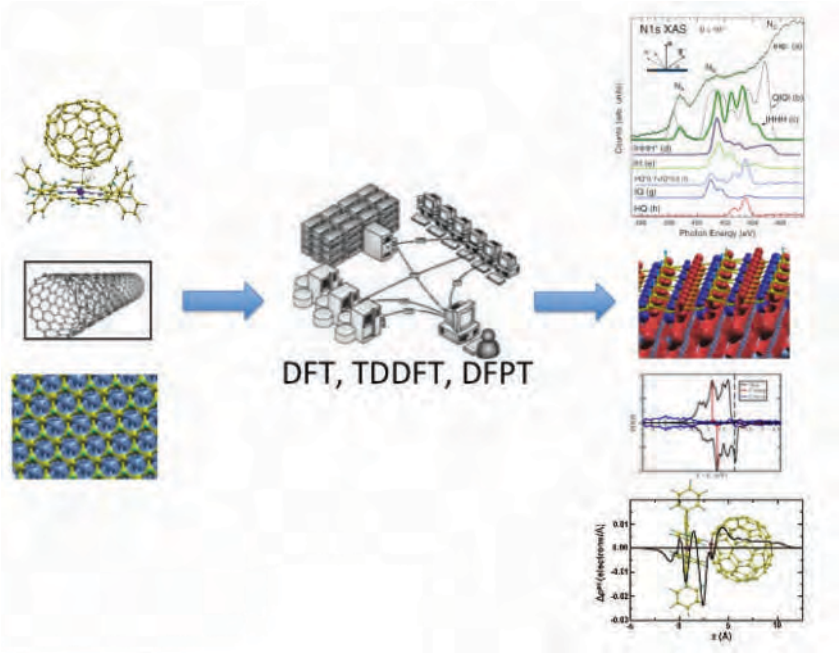
PRASENJIT GHOSH

Assistant Professor

Ph.D.: Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India
Post-doc.: Abdus Salam International Centre for Theoretical Physics, Trieste, Italy
Joining at IISER: September 2010
Email: pghosh@iiserpune.ac.in
URL: http://www.iiserpune.ac.in/~pghosh/

Computational Material Science

Research in our group involves exploring novel physics and chemistry at the nanoscale using theoretical tools. In particular we are interested in how properties (e.g. structural, electronic, vibrational, magnetic and chemical) change upon reducing size or lowering dimensionality (particularly in the nanoscale) and how these changes effect the phenomena associated with these low dimensional (e.g. nanowires, nanotubes, surfaces and clusters) materials. To address such issues we perform first principles calculations using quantum mechanical density functional theory (for ground state properties), density functional perturbation theory (for vibrational properties) and time dependent density functional theory (for excited state properties). We actively collaborate with experimental groups both at IISER Pune and outside.



Using the above methods, we try to achieve the following goals: (a) understand aspects of chemical bonding and microscopic couplings that are essential to the specific properties of materials, (b) obtain information about the atomistic structure and electronic states, which are often hard and sometimes inaccessible to experiments and (c) design new materials and/or modify existing materials to yield materials

with desired properties. We are primarily interested in materials with applications in heterogeneous catalysis, photocatalytic water splitting, thermoelectrics, etc. Further we are also involved in developing computational tools, which can be used to understand material properties.

Publications

Total number of publications: 18 **; Independent publications:** 9

Selected Publications

- Varghese, A.; **Ghosh, P.**; Datta, S. Cadmium Vacancy Minority Defects as Luminescence Centers in Size and Strain Dependent Photoluminescence Shifts in CdS Nanotubes**.** J. *Phys. Chem.* C 2014, 118, 21604-21613.
- **Ghosh, P**.; Camellone, M. F.; Fabris, S. Fluxionality of Au clusters at ceria surfaces during CO oxidation: relationships among reactivity, size, cohesion, and surface defects from DFT simulations. *J. Phys. Chem. Lett.* **2013,** ***4***, 2256-2263.
- Santra, S.; Hota, P. K.; Bhattacharyya, R.; Bera, P.; **Ghosh, P.;** Mandal, S. K. Palladium Nanoparticles on Graphite Oxide: A Recyclable Catalyst for the Synthesis of Biaryl Cores. *ACS Catalysis* **2013**, *3*, 2776-2789.
- Kaul, I.; Joshi, N.; Ballav N.; **Ghosh, P**. Hydrogenation of Ferrimagnetic Graphene on a Co Surface: Significant Enhancement of Spin Moments by C-H Functionality. *J. Phys. Chem. Lett.* **2012, *3***, 2582-2587.
- Joshi, N.; Ballav, N; **Ghosh, P.** Hydrogen-induced reversal of spin alignment in graphene supported on Ni(111) surface. *Phys. Rev.* B **2012**, *86*, 121411(R).

Teaching Contributions

Scientific Computing, Solid State Chemistry, Molecular Modeling in Chemistry, Computational Physics, Mathematical Methods

Awards and Recognitions

- Associate, Abdus Salam ICTP, Trieste, Italy from 2012-2016

Research Group

Doctoral and project students: Debnath Talukdar, Indu Kaul, Nandha Kumar, Niharika Joshi, Subrahmanyam Sappati

Past under-graduate students: C. Gaurav

SUJIT KUMAR GHOSH

Assistant Professor

Ph.D.: Indian Institute of Technology, Kanpur, India
Post-doc.: Kyoto University, Japan
Joining at IISER: June 2009
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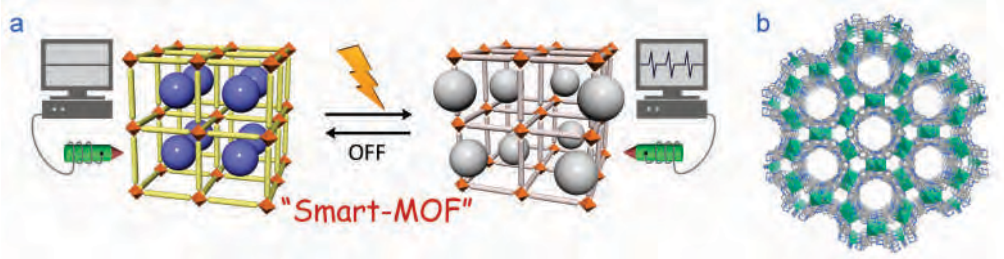
URL: http://www.iiserpune.ac.in/~sghosh/

Coordination Chemistry, Functional Porous Materials

The principal research focus of our laboratory is on the development of functional porous materials based on coordination polymers suited for applications in chemical industries, energy & environmental issues. Self assembly of predesigned organic building units and metal ions/clusters by engaging coordination affinity renders the desired multidimensional networked structure known as Metal-Organic Frameworks (MOFs) or Porous Coordination Polymers (PCPs). These materials have invoked interest in the fields of gas storage & separation, catalysis, ion recognition, chemical separation, ionic conductivity, sensing etc (Figure. a).

Carbon capture and storage (CCS) technology is seeking great attention in the recent years owing to the pressing issue of greenhouse gas emissions, especially CO_2. We have synthesized 3- dimensional metal-carboxylate porous MOFs with electron rich pore surface for selective CO_2 uptake over N_2, H_2, Ar, CH_4 gases. We have also utilized the open metal sites and secondary functionalities (like amine, hydroxy) present in MOFs for achieving selective CO_2 capture over potentially competing gases (Figure. b).



Chemical separation has great importance in industrial applications. In our lab flexible Zn(II) and carboxylate based MOFs have been developed for the separation of industrially vital monomers like benzene, *p*-xylene and styrene from the congener product streams.

Fuel cells have potential to produce energy in higher efficiencies with no environmental pollution. Zn(II) and oxalate based MOFs with high proton conductivity and chemical stability have been synthesized in our lab, which has potential to be utilized as proton exchange membrane in fuel cells.

MOF as a chemical sensor has been employed for multiple applications like explosive detection, *in vivo* neurotransmitter sensing and ion recognition. Chemically stable Zr(IV) and carboxylate based porous fluorescent MOF with free Lewis basic functional groups (like amine, pyridyl) has been developed for aqueous phase highly selective nitro explosive detection. A bio-compatible Zr(IV) and carboxylate based MOF based turn-on probe for detection of gasotransmitter H_2S in live cells has also been established in our lab.

Publications

Total number of publications: 62**; Independent publications:** 31

Selected Publications

- Nagarkar, S. S.; Unni, S. M.; Sharma, A.; Kurungot, S.; **Ghosh, S. K.** Two-in-one: Inherent Anhydrous and Water-assisted High Proton Conduction in a 3D Metal-Organic Framework. *Angew. Chem. Int. Ed.* **2014**, 53, 2638-2642.
- Mukherjee, S.; Joarder, B.; Manna, B.; Desai, A. V.; Chaudhari, A. K.; **Ghosh, S. K.** Framework-Flexibility Driven Selective Sorption of *p*-Xylene over Other Isomers by a Dynamic Metal-Organic Framework**.** *Sci. Rep.* **2014**, 4, DOI: 10.1038/srep05761.
- Joarder, B.; Mukherjee, S.; Chaudhari, A. K.; Desai, A. V.; Manna, B.; **Ghosh, S. K.** Guest-Responsive Function of a Dynamic Metal-Organic Framework with π-Lewis Acidic Pore Surface. *Chem. Eur. J.* **2014**, *20*, 15303 – 15308.
- Nagarkar, S. S.; Joarder, B.; Chaudhari, A. K.; Mukherjee, S.; **Ghosh, S. K.** Highly Selective Detection of Nitro-Explosive by a Luminescent Metal-Organic Framework. *Angew. Chem. Int. Ed.* **2013**, *52*, 2881-2885.
- Manna, B.; Chaudhari, A. K.; Joarder, B.; Karmakar, A.; **Ghosh, S. K.** Dynamic Structural Behavior and Anion-Responsive Tunable Luminescence of a Flexible Cationic Metal-Organic Framework. *Angew. Chem. Int. Ed.* **2013**, *52*, 998-1002.

External Grants

- Functional studies of novel inorganic organic hybrid frameworks with guest accessible sites. Funding Agency: DST-SERB (June 2012-May 2015).
- Development and functional studies of metal-organic polyhedral. Funding Agency: INSA Young Scientist start up grant (September 2014-August 2017).

Teaching Contributions

Introductory Inorganic Chemistry, Chemistry Lab II-Inorganic Chemistry, Main Group Chemistry, Transition Metal Chemistry, Advanced Inorganic Laboratory

Awards and Recognitions

- INSA Young Scientist Award, 2013, Alkyl Amines-ICT Foundation Day Young Scientist Award, 2013
- NASI-Young Scientist Award, 2012, Young Associate of the Indian Academy of Sciences, 2012
- DAE –BRNS Young Scientist Award, 2011
- JSPS Fellowship (Japan)2007-2009, Newton International Fellowship (UK) 2009

Research Group

Doctoral students: Sanjog S. Nagarkar, Biplab Joarder, Biplab Manna, Soumya Mukherjee, Avishek Karmakar, Partha Samanta, Aamod V. Desai

Project student: Arif Inamdar

Under-graduate student: Naveen Kumar

Past under-graduate students: Amitosh Sharma, Shweta Singh, Amrit Kumar Singh

HOSAHUDYA N. GOPI

Associate Professor

Ph.D.: Bangalore University, Bangalore, India
Post-doc.: Molecular Biophysics Unit, Indian Institute of Science, India
Post-doc.: Northwestern University, Evanston, USA
Post-doc.: Drexel University of College of Medicine, Philadelphia, USA
Assistant Professor: July 2007 –January 2013, IISER-Pune
Associate Professor: January 2013 – Present date, IISER-Pune
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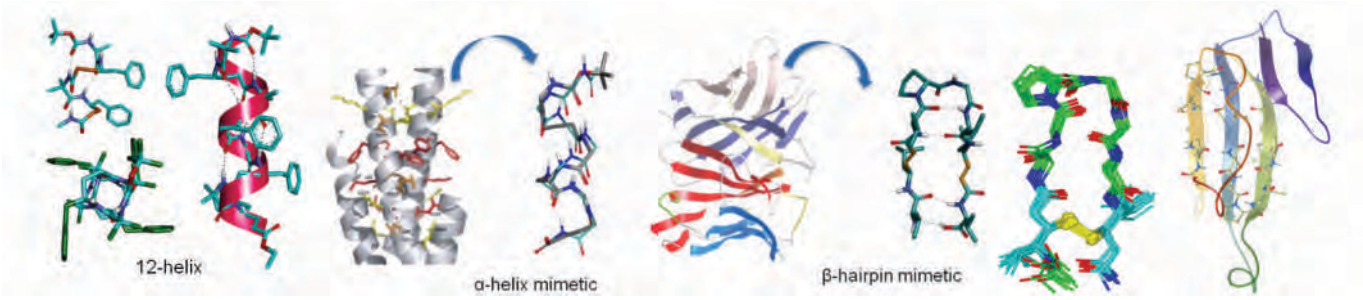
Foldamers, Peptidomimetics, Antibiotics and Biomaterials

The main research focus of this laboratory is on the synthesis and utilization of naturally occurring non-ribosomal amino acids along with the novel α–, β -and γ–amino acids towards the design of proteolytically stable Protein Secondary Structure Mimetics, Miniproteins, Peptidomimetics, Antibiotics and Biomaterials.

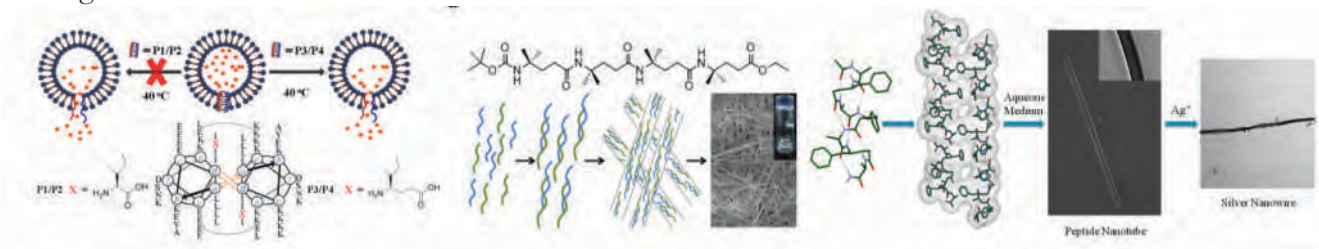
Mimicking Functional Epitopes of Proteins: Using hybrid peptide foldamers, we are exploring the possibilities to design functional protein epitope mimetics, which can be used as inhibitors for protein-protein interactions, protease inhibitors and synthetic vaccine candidates.



α ,γ-Hybrid peptides | Structural analogy with α-helix | β-Hairpins and multistranded β-sheets

Peptide Antibiotics: Besides the protein epitope mimetics, we are exploring short hybrid lipopeptides as novel antibacterial and antifungal candidates and the mechanism of action of these hybrid peptides.

Biomaterials: Efforts have also been undertaken to create novel biomaterials such as nanotubes, vesicles, nanofibers, polyhedrons, organogels and hydrogels from the proteolytically stable γ- and, α,γ-hybrid peptide foldamers and investigating the utility of these novel soft biomaterials as delivery vehicles, tissue culture and casting metal nanowires from metal ions.



γ-Amino acid mutated coiled-coils as mild temperature triggers | Thermoreversible organogels from γ-peptides | α,γ-Hybrid peptide nanotubes and their utility in casting silver nanowires

Publications

Total number of publications: 56**; Independent publications:** 21

Selected Publications

- Jadhav, S. V.; Misra, R.; **Gopi, H. N.** Foldamers to Nanotubes: Influence of Amino acid Side-chains in the Hierarchical Assembly of α,γ^4-Hybrid Peptide Helices *Chem. Eur.- J.* **2014**, *20*, 16523**.** (*Accepted as Very Important Paper*)
- Mali, S. M.; **Gopi. H. N.** Thioacetic acid/NaSH-mediated synthesis of *N*-protected amino thioacids and their utility in peptide synthesis. *J. Org. Chem.* **2014**, 79, 2377.
- Jadhav, S. V.; Singh, S. K.; Reja, R. M; **Gopi, H. N.** γ-Amino acid mutated α-coiled coils as mild thermal triggers for liposome delivery. *Chem Commun.* **2013**, *49*, 11065
- Shankar, S. S.; Benke, S. N.; Nagendra, N.; Srivastava, P. L.; Thulasiram, H.V.; **Gopi, H.N.** Self-assembly to function: design, synthesis, and broad spectrum antimicrobial properties of short hybrid *E*-vinylogous lipopeptides**.** *J. Med. Chem.* **2013**, *56*, 8468.
- Bandyopadhyay, A.; Jadhav, S. V.; **Gopi, H. N.** α/γ^4-Hybrid peptide helices: synthesis, crystal conformations and analogy with the α-helix. *Chem. Commun.* **2012**, *48*, 7170.

External Grants

- Investigation of gamma and hybrid gamma helical peptides as HIV-1 fusion inhibitors: Funding Agency: DST, India (May 2010-April 2013).
- Exploration of naturally occurring β-hydroxy γ-amino acids (statines) in the design of foldamers and biological active peptidomimetics: Submitted to SERB-DST, India.
- Exploring the Antimicrobial Activities of short ,α-γ Hybrid Lipopeptides: Submitted to CSIR, India.

Teaching Contributions

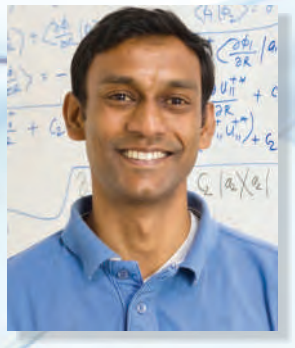
Introductory Organic Chemistry, Physical Organic Chemistry, Organic Synthesis I, Photochemistry, Chemistry Lab III- Organic Chemistry and Advanced Organic Laboratory

Research Group

Doctoral students: Mothukuri Ganesh Kumar, Sushil N. Benke, Rajkumar Misra, Anindita Adak, Rahi M. Reja, K. Veeresh, Rupal D. Bhaisare

Former Ph. D Students: Dr. Anupam Bandyopadhyay, Dr. Sandip V. Jadhav, Dr. Sachitanand M. Mali

Past under-graduate students: Mr. Kumar Saurav, Ms. Neha Agrawal, Mr. Sumeet K. Singh, Ms. Ankita Malik and Mr. Rupal D. Bhaisare



ANIRBAN HAZRA

Assistant Professor

Ph.D.: Princeton University, Princeton, USA
Post-doc.: Pennsylvania State University, University Park, USA
Joining at IISER: July 2011
Email: ahazra@iiserpune.ac.in
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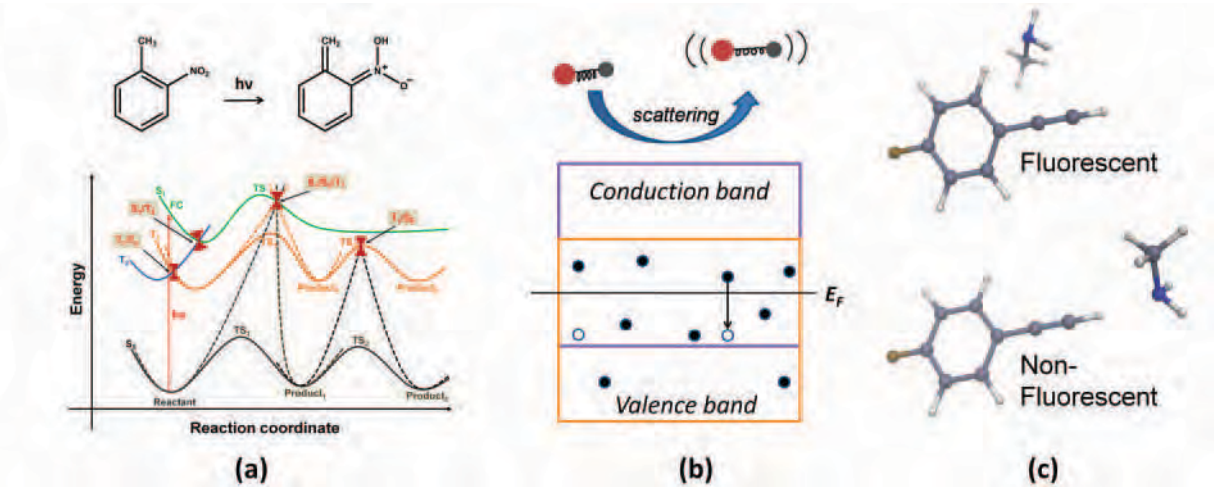
Theoretical and Computational Chemistry

The theme of our research is theoretical investigation of excited state molecular phenomena using quantum chemistry and nuclear dynamics methods. Excited state processes constitute a large class of phenomena in nature. Several of these phenomena like photoinduced electron transfer, photodissociation and florescence quenching occur at the ultrafast or femtosecond timescale and play important roles in living organisms and in atmospheric phenomena. The detailed mechanistic understanding of such processes is of basic scientific interest and is also important for its technological implications in solar-based renewable energy devices, particularly the conversion of solar energy to chemical energy.

The mechanism of photo-induced tautomerization of *o*-nitro toluene to its aci-nitro tautomer has been explored using *ab inito* electronic structure calculations. The reaction is found to proceed through a complex pathway, involving both singlet and triplet states. Methods for finding interesting topologies like a three-state conical intersections have been developed (Figure a).



The independent-electron surface hopping method has been implemented to study nonadiabatic phenomena during molecule-surface interactions. It is being applied to explain energy transfer to intra-molecular degrees of freedom during scattering of molecules from surfaces (Figure b).

The mechanism of fluorescence quenching in certain conformers of the weakly bound fluorophenylacetylene-methylamine complex in the gas phase is being investigated using electronic structure calculations (Figure c).

Publications

Total number of publications: 15**; Independent publications:** 3

Selected Publications

- Joshi, S.; Shukla, A.; Katiyar, H.; **Hazra, A.**; Mahesh, T. S. Estimating Franck-Condon factors using an NMR quantum processor. *Phys. Rev. A* **2014**, *90,* 022303.
- Malwal, S. R.; Gudem, M.; **Hazra, A.**; Chakrapani, H. Benzosultines as Sulfur Dioxide (SO_2) Donors. *Org. Lett.* **2013**, *15,* 1116-1119.

External Grants

- Development and application of theoretical methods for mechanistic understanding of ultrafast photoinduced molecular processes. Funding Agency: SERB-DST, India. (August 2012-July 2015).

Teaching Contributions

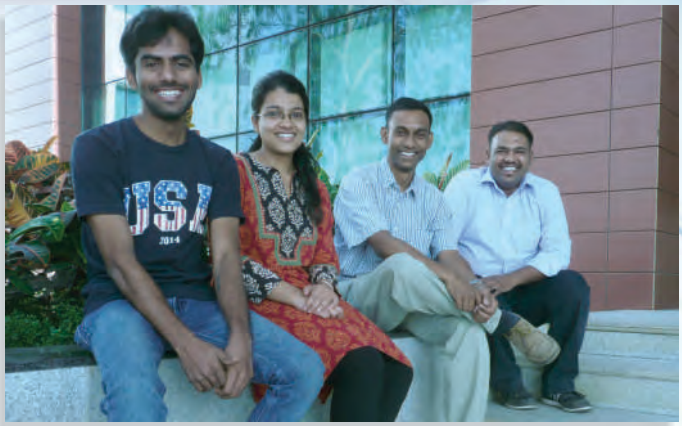
Symmetry and Group Theory, Quantum Chemistry

Research Group

Doctoral students: Avdhoot Datar, Mahesh Gudem, Meghna Manae

Under-graduate students: Khushboo Singh

Past under-graduate students: P Sudheer Kumar



PARTHA HAZRA

Associate Professor

Ph.D.: Indian Institute of Technology, Kharagpur, India
Post-doc.: Kyoto University, Japan (JSPS Fellow)
Assistant Professor: February 2008 – July 2014, IISER-Pune
Associate Professor: August 2014 – Present date, IISER-Pune
Email: p.hazra@iiserpune.ac.in
URL: http://www.iiserpune.ac.in/~p.hazra/

Photophysics and Biophysics

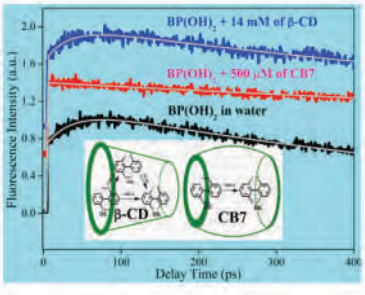
The main research focus of this laboratory is to study the excited state photophysics of fluorophores/drugs in molecular containers, various kinds of self-assembled organized structures as well as in biologically tailored systems.

Molecular containers have the ability to encase biologically relevant guests, and act as drug carriers, drug solubilizers, and drug stabilizers. The inclusion of the fluorescent guest into these nano-cavities is point of interest due to their altered excited state photophysics such as excited state proton transfer.

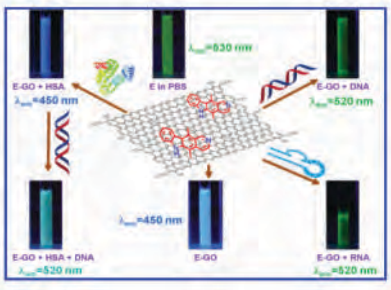
Graphene oxide molecular switching of ellipticine (E) has been utilized to probe its efficient loading onto graphene oxide (GO) and subsequent release to intra-cellular biomolecules like DNA/RNA.

Bio-molecular Interactions such as drug-DNA, drug-G-quadruplex DNA, drug-RNA and protein-DNA are explored by various biophysical techniques (fluorescence, CD, ITC etc.).

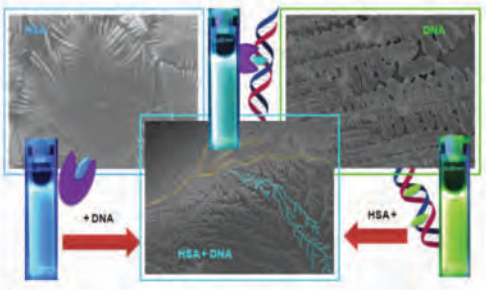
ESPT dynamics and Solvation Dynamics are explored by ultrafast spectroscopy such as TCSPC and femto-second fluorescence up-conversion techniques in bio-mimicking confined environments.



Modulation of ESPT Dynamics of $BP(OH)_2$ inside the molecular containers.



Fluorescence-switching of ellipticine in the presence of GO with various bio-macromolecules (HSA/ dsDNA /RNA).



A visible fluorescence switch of an eminent anti-carcinogen, ellipticine has been used to probe non-specific protein-DNA interaction.

Publications

Total number of publications: 43**; Independent publications:** 21

Selected Publications

- Kumar,V.; Sengupta, A.; Gavvala, K.; Koninti, R. K.; **Hazra, P.** Spectroscopic and Thermodynamic Insights into the Interaction between Proflavine and Human Telomeric G-Quadruplex DNA. *J. Phys. Chem. B,* **2014**, *118*, 11090–11099.
- Sengupta, A.; Gavvala, K.; Koninti, R. K.; Ballav, N.; **Hazra, P.** An Anticancer Drug to Probe Non-specific Protein-DNA Interactions. *Phys. Chem. Chem. Phys.* **2014**, 16, 3914-3917.
- Koninti, R. K.; Sengupta, A.; Gavvala, K.; Ballav, N.; **Hazra, P.** Loading of an Anti-cancer Drug onto Graphene Oxide and Subsequent Release to DNA/RNA: A Direct Optical Detection. *Nanoscale*, **2014**, 6, 2937-2944.
- Gavvala, K.; Sengupta, A.; Koninti, R. K.; **Hazra, P.** Femtosecond to Nanosecond Dynamics of 2, 2-Bipyridine-3,3-diol inside the Nano-Cavities of Molecular Containers. *Phys. Chem. Chem. Phys.* **2014**, 16, 933 – 939.
- Sengupta, A.; Singh, R. K.; Gavvala, K.; Koninti, R. K.; Mukherjee, A.; **Hazra, P.** Urea Induced Unfolding Dynamics of Flavin Adenine Dinucleotide (FAD): Spectroscopic And Molecular Dynamics Simulation Studies from Femto-second to Nano-Second Regime. *J. Phys. Chem. B,* **2014**, 118, 1881-1890.

External Grants

- New insight of flavin-aptamer recognition process with the help of biophysical studies. Funding Agency: CSIR, Govt. of India (January 2012-December 2015).
- Photoinduced electron transfer rate (between flavins and aromatic amino acids) in nanocavity of proteins versus bulk water. Funding Agency: DST, Govt. of India (January 2010- January 2013).

Teaching Contributions

Basic Physical Chemistry, Symmetry and Group Theory, Advanced Physical Chemistry, Photochemistry

Awards and Recognitions

- Awarded *Japan Society of Promotion of Science (JSPS)* fellowship in 2005 for pursuing post-doctoral research in Japan

Research Group

Graduate Students: Krishna Gavvala, Raj Kumar Koninti, Sagar Satpathi, Bibhisan Roy

Past under-graduate students: Vivek Kumar, Anup Ingole

Past graduate Student: Dr. Abhigyan Sengupta (Presently, JILA post-doctoral fellow in the University of Colorado, Boulder USA)

SRINIVAS HOTHA

Associate Professor

Ph.D.: Osmania University (worked at IICT, NCL), Hyderabad, India
Post-doc.: Rockefeller University, New York, USA
Previous positions: Scientist-C then E1, National Chemical Laboratory, Pune
Joining at IISER: November 2010
Email: s.hotha@iiserpune.ac.in
URL: http://www.iiserpune.ac.in/~s.hotha

Chemical Glycobiology

In chemical glycobiology laboratory, we are interested in developing catalytic tools for glycosylation. Alkynyl glycosides were found to be excellent for carrying-out glycosidations in a stereo- and sometimes regioselective manner. The gold catalysis method developed in the group is complementary to some of the already existing methods and is found to be advantageous for the synthesis of glycopolypeptides, glycopolymers, glycomimetics, oligosaccharides and host of other molecules where glycans are represented.

Quite recently gold-catalysis repertoire has been effectively utilized for the synthesis of various carbohydrate epitopes present on the cell surfaces of infectious bacteria. The group is actively involved in the synthesis of arabinogalactan portion of the mycobacterial cell surface. We developed methods for the stereoselective syntheses of all four furanosides in a catalytic manner taking cue from mycobacteriology.

Biophysical studies on glycans: Most of the cell surface oligosaccharides are attached to either lipids or peptides to make them functional. Specifically, mycobacteria have a unique glycolipid comprising arabinose residues are in the furanosyl form and the terminal residues are esterified with cyclopropanated mycolic acids. We are trying to understand the structure-property relationship of the glycolipid composition of *Mycobacterium tuberculosis*. Understandings from the biophysical studies on glycolipids, shall be extended to develop biosensor for non-invasive diagnosis of Tuberculosis.

Ligation Methods: In the era of chemical biology and material science, novel ligation methods are in great demand. Significant developments around the most popular 'click'chemistry between azide and alkyne has shown its benefits in variety of fields. The recent addition to the list of 'click' protocols is the chemistry of *s*-tetrazines. We are currently developing *s*-tetrazine based strategies for the ternary and quaternary conjugates which will be utilized further in chemical biology experiments.

Publications

Total number of publications: 52**; Independent publications:** 43

Selected Publications

- Thadke, S. A.; Mishra, B.; **Hotha, S.** Gold(III)-Catalyzed Glycosidations for 1,2-*trans* and 1,2-cis Furanosides. *J. Org. Chem.* **2014**, 79, 7358-7371.
- Islam, M.; Tirukoti, N. D.; Nandi, S.; **Hotha, S.** Hypervalent Iodine Mediated Synthesis of C-2 *deoxy* Glycosides and Amino Acid Glycoconjugates. *J. Org. Chem.* **2014**, 79, 4470-4476.
- Rao, B. V.; Dhokale, S.; Rajamohanan, P.; **Hotha, S.** A Tetrazine Templated Method for the Synthesis of Ternary Conjugates. *Chem. Commun.* **2013**, 49, 10808-10810.
- Thadke, S. A.; Mishra, B.; **Hotha, S.** Facile Synthesis of β- and α- Arabinofuranosides and Application to Cell Wall Motifs. *Org. Lett.* **2013**, 15, 2466-2469..
- Kayastha, A. K.; **Hotha, S.** Versatile Gold catalyzed Trans-glycosidation Ambient Temperature *Chem. Commun.* **2012**, 48, 7161-7163.

External Grants

- Cascade glycosylations: A Novel Strategy for Carbohydrate Epitopes and Glycoarrays - Funding Agency: DST, India (Feb 2011-Dec 2016).
- Glycochemical studies of Mycobacterial Arabinoomycolate. Funding Agency: Indo-French Co-operation for Promoting Advanced Scientific Research (IFCPAR) India (April 2014- March 2017). [In collaboration with Prof. Theirry Benvegnu (France) and Prof. Pankaj Mandal (IISER Pune)]
- Tailoring Glycosylphosphatidylinositol Substrates and Substrate Minmetics to Study Host-Pathogen Interactions (Jan 2015-Dec 2017). [In collaboration with Prof. Sneha Sudha Komat (JNU, India)]

Teaching Contributions

Organic Synthesis 1, Organic Synthesis 2, Medicinal Chemistry, Separation Principles and Techniques, Organic Chemistry Laboratory

Awards and Recognitions

- CDRI Award for Excellence in Drug Research (2014)
- Bronze Medal of Chemical Research Society of India (2015)

Research Group

Doctoral and project students: Boddu Venkateswara Rao, Maidul Islam, Bijoyananda Mishra, Mahesh Neralkar, Ganesh Shinde, Sujit Manmode

Post-doctoral Fellows: Madhuri Vangala, Sandip Pasari, Dinanath Phulse

Past doctoral students: Shivaji A. Thadke, Abhijeet Kayastha, Ashif Y. Shaikh, Srinivasa Rao Vidadala, Suresh Kumar Gopalsamy, Ashish Tripathi, Sudhir Kashyap, Sushil Kumar Maurya, Ramakrishna I. Anegundi

Past under-graduate students: Iti Kapoor, Ravi Raja

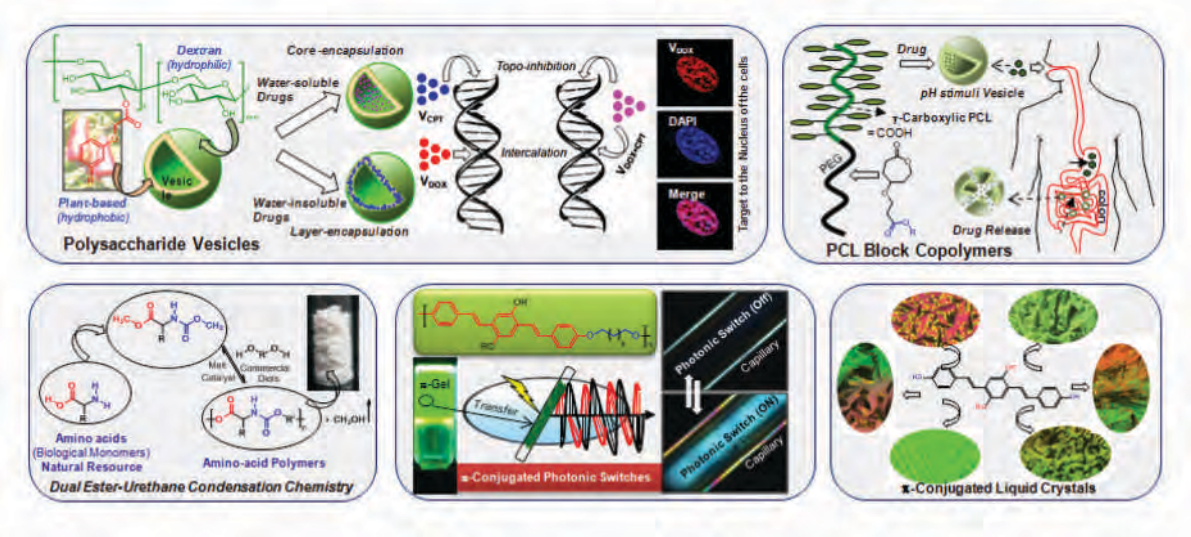
M. JAYAKANNAN

Associate Professor

Ph.D.: Indian Institute of Science, Bangalore, India
Post-doc.: Technical University of Eindhoven, The Netherlands
Previous position: Polymer Scientist, GE Plastics, JFWTC, Bangalore
Previous position: Scientist, NIIST (CSIR) Trivandrum, India
Assistant Professor: December 2007 – March 2010, IISER-Pune
Associate Professor: March 2010 – Present date, IISER-Pune
Email: jayakannan@iiserpune.ac.in
URL: http://www.iiserpune.ac.in/~jayakannan/

Polymer Science

The research group has been working in the area of polymer science for the past 12 years and the group's work is primarily focused on design and development of new macromolecular systems for application in electronics and biomaterials.



Polymers based drug delivery is an important tool for the administration of drugs in cancer treatment. New generation of enzyme responsive polysaccharides-dextran nano-vesicles, pH responsive functionalized polycaprolactone (PCL) block copolymers and shape transformable thermo-responsive amphiphilies were developed. These scaffolds were utilized for loading and delivering of multiple anticancer drugs to achieve synergistic killing of cancer cells.

Eco-friendly synthetic approaches are important for cleaner and environmental friendly production of polymer materials. *A novel melt transurethane* process was developed for commercial important thermoplastics polyurethanes. Recently, a new *dual ester-urethane melt condensation methodology* was developed for biological monomers- amino acids that produced new classes of biodegradable thermoplastics under eco-friendly and solvent free approach.

Polymers for electronics are developed based on π-conjugated OPV molecules that self-organized to produce three dimensional supra-structures such as chlolestric liquid crystalline (LC) mesophases. π-Conjugated polymer anisotropic organogels were achieved in segmented OPV polymers that facilitated the

demonstration of first example for π-conjugated photonic switches (or photonic wave plates). Thermo-responsive photonic switches were constructed for the temperature range of 25 to 160 °C.

Publications

Total number of publications: 73**; Independent publications:** 56

Selected Publications

- Pramod, P. S.; Shah, R.; Sonali, C.; Balasubramanian, N.; **Jayakannan, M.** Polysaccharide Nano-vesicular Multidrug Carrier for Synergistic Killing of Cancer Cells, *Nanoscale*, **2014**, *6*, 11841- 11855.
- Goel, M.; Narasimha, K.; **Jayakannan, M.** Helical Self-assemblies of Segmented Poly(phenylene-vinylene)s and their Hierarchical Donor-Acceptor Complexes. *Macromolecules*, **2014**, *47*, 2592-2603.
- Balamurugan, A.; Vikash Kumar; **Jayakannan, M.** Carboxylic Distilbene Fluorescent Polymer Chemosensor for Temperature, Metal-ion and Biomolecule, *Chem. Commun*. **2014**, *50*, 842-845.
- Bapurao Surnar; **Jayakannan, M.** Stimuli-responsive Polycaprolactone Vesicles for Dual Drug Delivery under GI Tract, *Biomacromolecules*, **2013**, *14,* 4377-4387.
- Anantharaj, S.; **Jayakannan, M.** Polymers from Amino acids: Development of Dual Ester-urethane Melt Condensation Approach and Mechanistic Aspects. *Biomacromolecules,* **2012**, *13*, 2446- 2455.

External Grants

- In the last ten years, more than 5 projects were funded by DST, New Delhi, India
- Design and Development of Amino acid Based Polymer Scaffolds for Drug Delivery. Funding Agency: SERB-DST, India (August 2014-July 2017).
- Development of Functional π-Conjugated Polymers for Photonic Applications. Funding Agency: SERB-DST under Special Initiative, India (Just Approved).

Teaching Contributions

Polymer Chemistry, Self-assembly in Chemistry, Separation Principles and Techniques, Introductory Physical Chemistry

Awards and Recognitions

- Chemical Research Society of India (CRSI) Bronze Medal 2014
- TWAS Young Affiliates-2010
- CSIR Young Scientist Award 2007 in Chemical Sciences

Research Group

Doctoral students: Smita Kashyap, P. S. Pramod, S. Anantharaj, Bapurao Surnar, Rajendra Aluri, Karnati Narasimha, Bhagyashree Kulkarni, Sonashree Saxena, Nilesh Deshpande

Under-graduate students: Thameez Mohammed, Maitreyee Mhatre

Past Doctoral students: Drs. Mahima Goel, A. Balamurugan, M. Jinish Antony, P. Anilkumar, Amrutha Rajan and Deepa Puthanparambil

Past under-graduate students: Harpreet Singh, Anuj Bisht, Uma Sridhar, Vikash Kumar

JEET KALIA

Assistant Professor

Ph.D.: University of Wisconsin-Madison, USA
Post-doc.: National Institutes of Health, Bethesda, USA
Joining at IISER: June 2013
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URL: http://www.iiserpune.ac.in/~jeet/

Chemical Biology: Ion channels, Lipids, and Bioconjugation

There are three major research foci of this laboratory: ion channel biology, lipid biology, and bioconjugation. All projects in the lab are inherently interdisciplinary and combine disciplines as wide-ranging as electrophysiology, molecular biology, protein expression and purification, protein chemistry and organic synthesis.

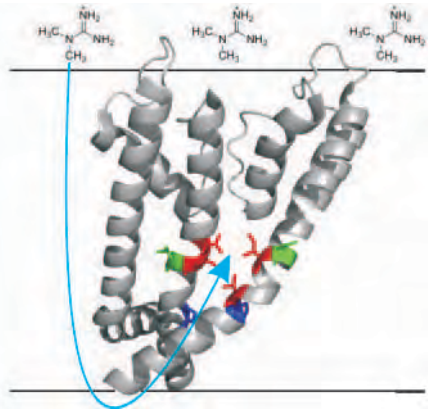

Figure 1. Our work on the inhibition of Kv channels by guanidine compounds resulted in elucidation of the binding site of these drugs on the channel.

Ion Channel Biology: Our work on ion channels is focused on tetrameric cation channels, especially voltage-activated potassium (Kv) channels, voltage-activated sodium (Nav) channels, and Transient Receptor Potential (TRP) ion channels. We utilize electrophysiological approaches to elucidate how these ion channels open and close in response to specific stimuli such as voltage, hot or cold temperatures, small chemical ligands and peptide toxins produced by venomous animals. Moreover, we are developing synthetic small molecules and peptide ligands that can specifically modulate the activity of these ion channels, thereby serving as mechanistic tools and also potentially serve as therapeutic agents (an example from our work that demonstrated the mechanism of inhibition of Kv channels by guanidine compounds is depicted in Figure 1). Our recent work on targeting Nav channels for anti-epileptic drug development resulted in the discovery of a novel triazole compound that attenuates epileptic seizures in rodents (ACS Chem. Biol. **2014** 9(5):1204-1212).

Lipid Biology: In comparison to proteins and nucleic the biological roles of lipids is poorly understood. The lack of powerful methods for studying lipids in cells is proving to be a major impediment in unraveling the roles of lipids in various cellular processes. To address this challenging problem, we are developing chemical biology based methods that will enable cellular incorporation of lipids possessing subtly-modified head groups endowed with elaborated function. Such modified lipids will serve as "lipid mutants" for studying the biology of lipids much in the same way protein mutants have contributed tremendously to protein biology. Our lipid mutants will help

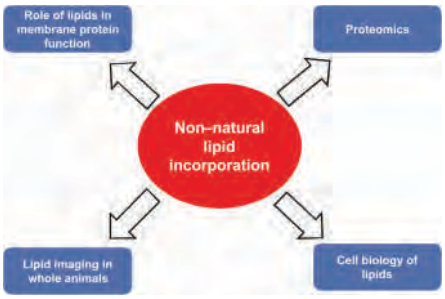

Figure 2. Applications of our proposed approach for introducing non natural lipids in cells.

address questions on the roles of lipids in several aspects of lipid and membrane biology including membrane protein function, membrane proteomics, cell biology of lipids and lipid imaging in both cells in culture and also in live animals (Figure 2).

Bioconjugation: Recent breakthroughs in chemical biology have enabled the development of selective methods of covalently modifying proteins. These bioconjugation approaches have been utilized for a host of applications including imaging of proteins in cells and live animals, diagnostic applications, and also for the discovery of interacting partners of proteins in cells. Despite all this progress, two major limitations remain: 1) Several existing bioconjugation linkages (for example, maleimides for thiol bioconjugation) are susceptible to hydrolysis and lack stability 2) The rates of formation of bioconjugates are too slow to enable precise spatiotemporal applications in cells. To address these limitations, we are developing new methods of bioconjugation that proceed rapidly and result in stable linkages.

Publications

Total number of publications: 15**; Independent publications:** 2**; Patent:** 1(U.S.)

Selected Publications

- **Kalia, J**., Milescu, M., Salvatierra, J., Wagner, J., Klint, J. K., King, G. F., Olivera, B. M., and Bosmans, F. From foe to friend: Using animal toxins to investigate ion channel function. *J. Mol. Biol.* **2014**, In press.
- Gilchrist, J., Dutton, S., Diaz-Bustamante, M., McPherson, A., Olivares, N., **Kalia J.**, Escayg, A., and Bosmans, F. Nav1.1 modulation by a novel triazole compound attenuates epileptic seizures in rodents. *ACS Chem. Biol.* **2014**, 9, 1204-1212.
- Marshall, C., Agarwal, N., **Kalia, J.**, Grosskopf, V., McGrath, N., Abbott, N. L., Raines, R. T., and Shusta, E. V. Facile chemical functionalization of proteins through intein-linked yeast display. *Bioconjugate Chem.* **2013**, 24, 1634-1644.
- **Kalia, J.** and Swartz, K. J. Elucidating the mechanism of action of a classical drug: Guanidine compounds as inhibitors of voltage-gated potassium channels. *Mol. Pharmacol.* **2011**, 80, 1085-1095.
- **Kalia, J.** and Raines, R. T. Hydrolytic stability of hydrazones and oximes. *Angew. Chem. Int. Ed. Engl.* **2008**, 47, 7523-7526.

Teaching Contributions

Introductory Biology Laboratory, Medicinal Chemistry, Advanced Organic Chemistry Laboratory

Awards and Recognitions

- NINDS competitive postdoctoral fellowship by NIH, U.S.A. for a period of 3 years (2009-2012).
- President's silver medal for topping the graduating Integrated M.Sc. class at IIT Kharagpur (2002).

Research Group

Doctoral and project students: Rahul Nisal, Debayan Sarkar, Shaila Kulkarni and Chitra Shanbhag

Under-graduate students: Sushma Tejashri

SHABANA KHAN

Assistant Professor

Ph.D.: Indian Institute of Technology, Delhi, India
Post-doc.: University of Göttingen, Germany
Post-doc.: Max-Planck-Institute for Coal Research, Mülheim, Germany
Previous position: Senior Scientist, BPCL R&D centre, India
Joining at IISER: March 2013
Email: shabana@iiserpune.ac.in
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Inorganic Chemistry and Catalysis

The main research focus is on developing novel silicon based frustrated Lewis pairs (FLPs) and utilization of these Si-based FLPs to activate small molecules such as H_2, CO_2, P_4, C_2H_4 and to use them as catalysts for organic reactions. We have been involved in synthesizing examples of N-heterocylic silylenes as base component along with various boron, carbon and silicon based Lewis acids to obtain new families of FLPs.

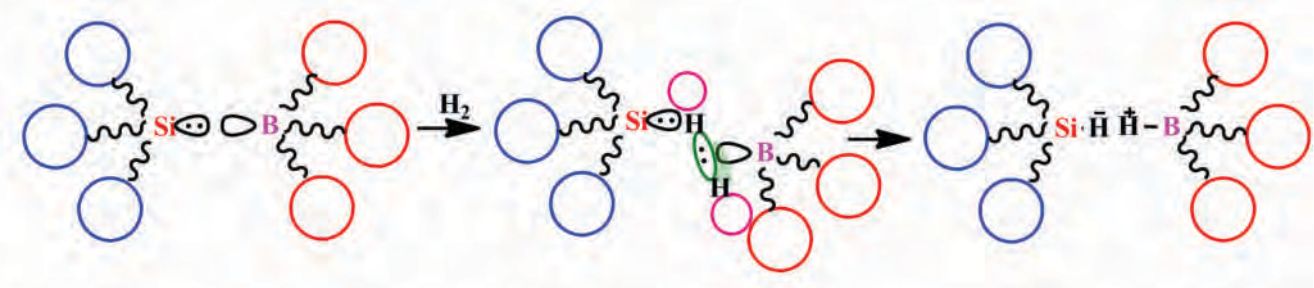


Figure 1. Activation of H_2

Gold(I) complexes and their catalytic activity is another topic of interest. In recent years gold(I) complexes have shown excellent catalytic activity in many homogeneous transformations involving C-C-π systems (alkenes, dienes, alkynes, allenes, arenes) towards the attack of a large variety of nucleophiles. In this view, we have been involved in developing PNP and PNB based Au^+ complexes which can be further used in catalytic reactions. Utilizing a PNP system, a dimeric Au-monocation has been formed while with a PNB system monomeric Au-monocation was achieved. The luminescent properties and catalytic activities of these newly synthesized Au^+ complexes are currently been explored in our laboratory.

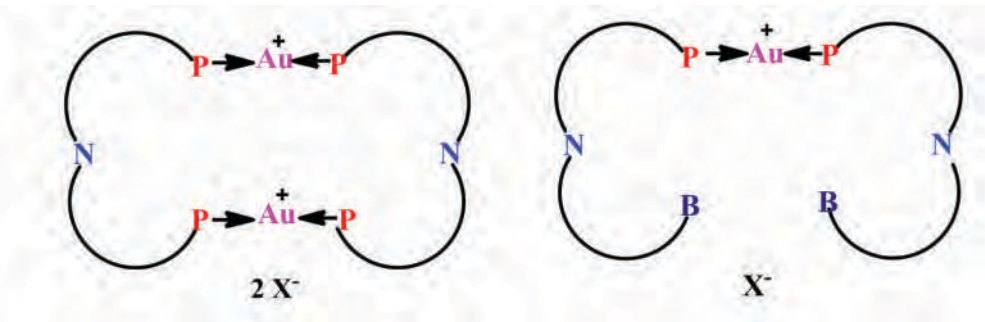


Figure 2. PNP and PNB framework based Au^+ cations

Publications

Total number of publications: 18

Selected Publications

- **Khan, S.**, Gopakumar, G., Thiel, W., Alcarazo, M. Stabilization of Dicoordinate $[GeCl]^+$ Cation by Simultaneous σ- and π-Donation from a Monodentate Carbodiphosphorane *Angew. Chem. Int. Ed.* **2013**, *52*, 5644-5647.
- **Khan, S.**, Michel, R., Sen, S. S., Roesky, H. W., Stalke, D. A P_4 Chain and Cage from Silylene-Activated White Phosphorus *Angew. Chem. Int. Ed.* **2011,** *50*, 11786–11789.
- **Khan, S.**, Michel, R., Dieterich, J. M., Mata, R. A., Roesky, H. W., Demers,, J.-P., Lange, A., Stalke, D. Preparation of RSn(I)–Sn(I)R with Two Unsymmetrically Coordinated Sn(I) Atoms and Subsequent Gentle Activation of P_4 *J. Am. Chem. Soc.* **2011**, *133*, 17889–17894.
- Sen, S. S., **Khan, S.**, Roesky, H. W., Kratzert, D., Meindl, K., Henn, J., Stalke, D., Demers, J.-P., Lange, A. Zwitterionic Si-C-Si-P and Si-P-Si-P Four-Membered Rings with Two- Coordinate Phosphorus Atoms *Angew. Chem. Int. Ed.* **2011,** *50*, 2322–2325.
- **Khan, S.**, Singh, J. D., Mahajan, R. K., Sood, P. Synthesis of Lariat Organochalcogenoethers Based on Azacalix[3]arenes for the Potentiometric Detection of UO_2^{2+} Ions *Tetrahedron Letters* **2007,** *48,* 3605–3608.

External Grants

- Introduction of Silylene in Frustrated Lewis Pair Chemistry and their Reactivity toward Small Molecules. SERB-DST, India (September 2014-August 2017).

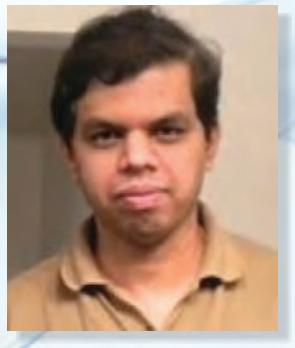
Teaching Contributions

Chemistry Lab II-Inorganic Chemistry, Main Group Chemistry, Transition Metal Chemistry

Research Group

Doctoral students:

Mr. Shiv Pal, Ms. Neha Kathewad



RAGHAVENDRA KIKKERI

Assistant Professor

Ph.D.: Weizmann Institute of Science, Israel
Post-doc.: ETH Zurich, Switzerland
Post-doc.: MPIKG. Berlin, Germany
Post-doc.: University of California, San Dieg, USA
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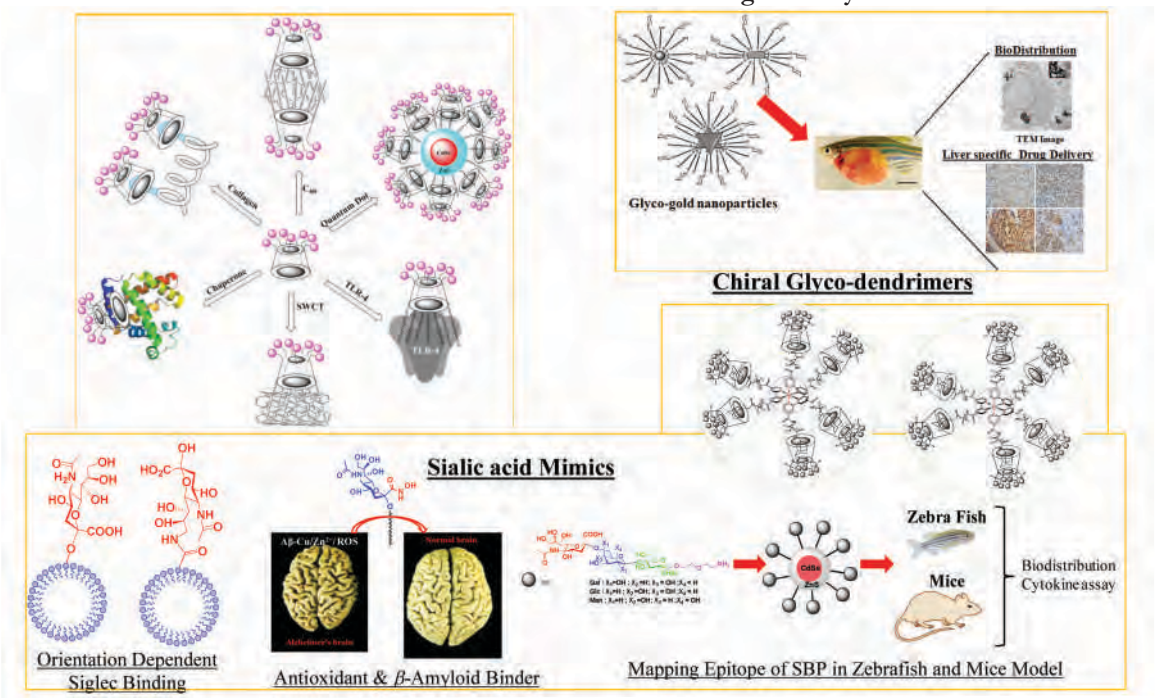
Glycochemistry, Glyconanotechnology and Glycobiology

Carbohydrates play an important role in many biological systems by virtue of their lectins which recognize them. Carbohydrate-lectin interactions are involved in expansively diverse biological processes which include embryonic development, intracellular trafficking, cell-cell recognition, cell activation, cell adhesion, cell homing, endocytosis, phagocytosis, inflammation, tumor cell metastasis, and apoptosis. One main drawback for investigating carbohydrate-lectin interactions is their weak affinity to bind, which will require enhanced tools to analyze carbohydrate-lectin interplay. So far, three promising strategies have emerged from our studies: (1) designing multivalent glyco-probes using cyclodextrin templates and their utilization towards amplifying carbohydrate mediated targeting, self-assembly, and remote actuation of particles to treat tumors in cancer models; (2) developing biomimetic carbohydrate strategies to modulate carbohydrate-protein interactions and (3) shape, chiral and symmetric dependent amplification of carbohydrate-protein interactions.

Schematic Representation of Selected Applications of Glyco-cyclodextrin

Influence of Glyco-nanoparticles Shape on Targeting and Drug Delivery *in Vitro* and *in Vivo*



Publications

Total number of publications: 31**; Independent publications:** 10

Selected Publications

- Yadav, R.; **Kikkeri, R.** Exploring the effect of sialic acid orientation on ligand-recentor interactions, *Chem. Commun*. **2012**, 48, 7265-7267.
- Yadav, R.; **Kikkeri, R.** Carbohydrate functionalized iron(III) complexes as biomimetic siderophores, *Chem. Commun*. **2012**, 48, 1704-1706.
- Bavireddi, H.; Bharate, P.; **Kikkeri, R.** Use of Boolean and fuzzy logics in lactose glycocluster research, *Chem. Commun*. **2013**, 49, 9185-7.
- Bavireddi, H.; Bharate, P.; **Kikkeri, R.** Probing carbohydrate-carbohydrate interactions by photos-witchable supramolecular glycoclutures. *Chem. Commun*. **2013**, 49, 3988-90.
- Gade, M.; P. Khandelwal,; S. Sangabathuni,; H. Bavireddi,; R. V. Murthy,; P. Pddar,; **R. Kikkeri**, Supramolecular scaffold on gold surface orients carbohydrates to sense proteins and macrophages. *Chem. Eur-J*, **2014**, Accepted.

External Grants

- DST-MPG Partner group: Carbohydrate capepd nanoparticles as tumor specific drug delivery system from 2011 to 2016**.**
- Department of Energy (DAE): Chiral lanthanide carbohydrate clusters for studying carbohydrate-protein interactions from 2011 to 2014.
- DST Indo-Israel S & T: Directed Assembly of Poly-nuclear Ru(II) Complexes On Carbon Nanostructures : A Prospective Organic Photovoltaic Cell From 2011 to 2013**.**

Teaching Contributions

Introductory Organic Chemistry, Advanced Organic Laboratory, Chemical Biology, Bioorganic chemistry

Awards and Recognitions

- DAE young research award

Research Group

Doctoral and project students: Rohan Yadav, Sivakoti Sangabhatuni, Harikrishna Bavireddi, Madhuri Gade, D. S. Chethan, Balamurugan

Under-graduate students: Phaneendra, Catherina Alex

Post doctoral students : R.V Murthy, Preeti Chaudhari

Past students: Priya bharate, Dr. Shadab Ali Khan

PANKAJ MANDAL

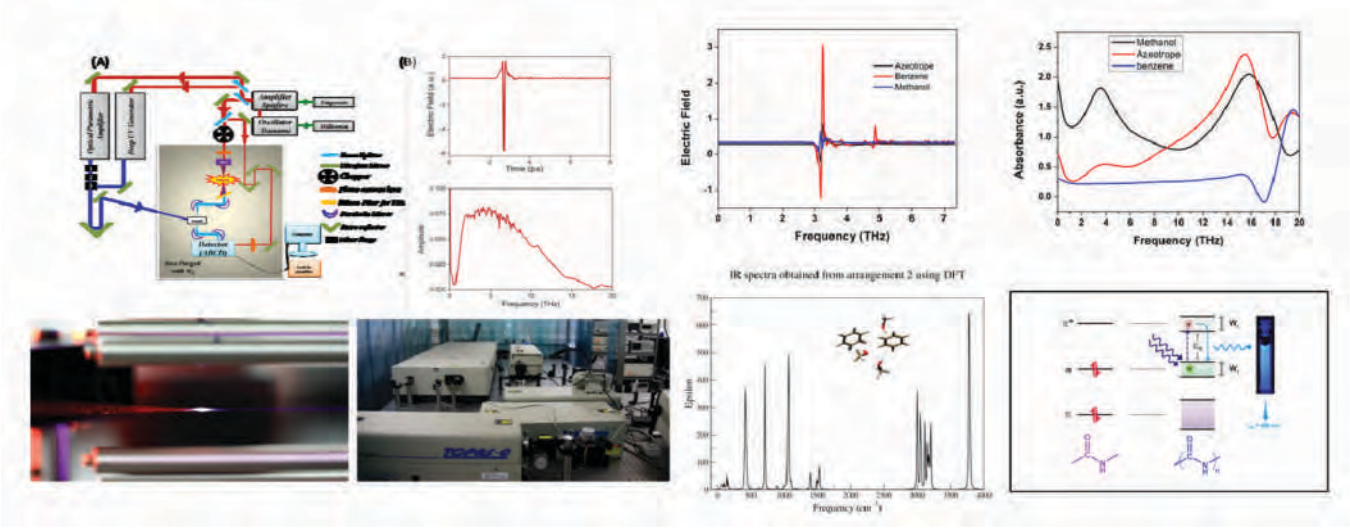
Assistant Professor

Ph.D.: Indian Institute of Science, Bangalore, India
Post-doc.: Rowland Institute @ Harvard, Cambridge, MA, USA
Post-doc.: Kansas State University, Manhattan, KS, USA
Joining at IISER: August 2010
Email: pankaji@iiserpune.ac.in
URL: http://www.iiserpune.ac.in/~pankaj/

THz Spectroscopy and Ultrafast Dynamics

The main research focus of this laboratory is on studying ultrafast dynamics in small molecules, biomacromolecules and nanomaterials. We employ ultrafast pump-probe technique where both pump and probe can be varied from THz to deep ultraviolet.

Broad band THz spectrometer has been built in our laboratory. Broadband THz pulse of sub-picosecond duration is produced from a four-wave-mixing process in air-plasma. We have successfully implement "Air Biased Coherent Detection" scheme for broadband detection. We have achieved a bandwidth of ~20 THz in our spectrometer. Such set-up for carrying out ultra-broadband THz spectroscopy is available only in few laboratories in the whole world, and is built for the first time in India. An experimental set-up for "optical pump-THz/white light probe Spectroscopy" has already been built. This set-up will enable probing a time-dependent (transient) event using either a broadband THz or a broadband white light (WL) as probe. A temporal resolution of 50 femto-second (fs) can be achieved.



Methanol-Benzene Azeotrope have been studied using our THz spectrometer and molecular dynamics simulation (in collaboration with Dr. Arnab Mukherjee) to evaluate the delicate balance of intermolecular interactions between molecules involved which lead to the formation of azeotropic mixture.

The origin of blue emission in Proteins has been studied. Our spectroscopic study of serum proteins reveals that the blue-green emission is, most likely, a property of protein monomer. Evidences suggest that semiconductor-like band structure of proteins with the optical band-gap in the visible region is possibly the origin of this phenomenon.

Publications

Total number of publications: 12**; Independent publications:** 1

Selected Publications

- Blue emission in proteins, Sohini Sarkar, Abhigyan Sengupta, Partha Hazra and **Pankaj Mandal**, arXiv:1404.6859 (2014).

External Grants

- Glycochemical Studies on Mycobacterial Arabinomycolate (with Dr. Srinivas Hohta, (IISER, Pune) Prof. Thierry, Benvegnu and colleagues (Ecole Nationale Supérieure de Chimie de Rennes)). Funding Agency: IFCPAR/CEFIPRA (February 2014- January 2017).

Teaching Contributions

Physical Chemistry (CHM 102), Chemistry Lab I-Physical Chemistry, Fundamentals of Molecular Spectroscopy, Advanced Molecular Spectroscopy, Symmetry and Group Theory

Research Group

Doctoral students: Sohini Sarkar, Y G Reddy, Sneha Banerjee, Avinash Warankar

M. JEGANMOHAN

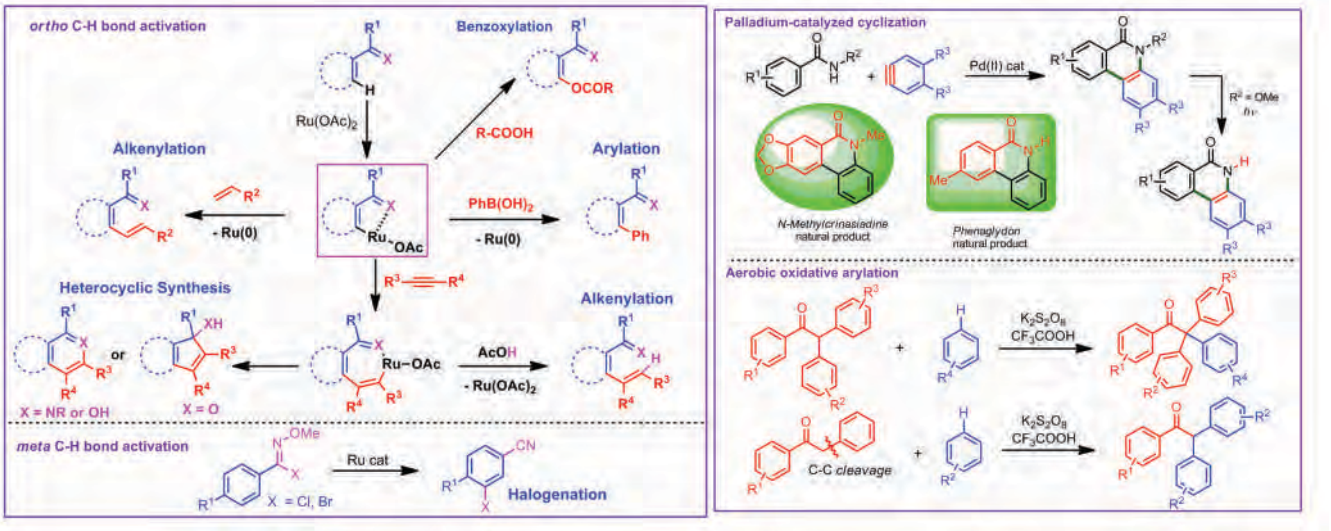
Assistant Professor

Ph.D.: National Tsing Hua University, Hsinchu, Taiwan
Post-doc.: National Tsing Hua University, Hsinchu, Taiwan
Post-doc.: Ludwig-Maximilians-Universität, Munich, Germany
Joining at IISER: November 2010
Email: mjeganmohan@iiserpune.ac.in
URL: http://www.iiserpune.ac.in/~mjeganmohan/

Organometallic and Organic Chemistry

The main research focus of this laboratory is the development of highly efficient, easily accessible and environmentally friendly organic transformations by using metal complexes as catalysts.

C-H Bond activation: Construction of chemical bonds via metal-catalyzed chelation-assisted C-H bond activation of aromatics, heteroaromatics and alkenes followed by functionalization with nucleophiles or electrophiles is a powerful tool in organic synthesis. This type of functionalization is highly atom-economical and environmentally friendly. Recently, we have developed several new synthetic methodologies for the C-H bond functionalization of aromatics, heteroaromatics and alkenes in the presence of ruthenium and palladium complexes as catalysts (Figure a). By using the present protocol, various substituted alkene derivatives, *ortho* benzoxylated aromatics, *ortho* arylated aromatics, *meta* halogenated benzonitriles and heterocycles were synthesized.



sp^3 C-H Bond α-arylation of substituted ketones: We have demonstrated a metal-free aerobic oxidative dehydrogenative α-arylation at the sp^3 C-H bond of substituted ketones with aromatics or heteroaromatics in the presence of $K_2S_2O_8$ giving hindered symmetrical and unsymmetrical benzopinacolone derivatives under the mild reaction conditions. On the other hand, benzyl ketones reacted with aromatics providing α-diarylated ketones through carbon-carbon bond cleavage. The reaction was carried out at room temperature under an air atmosphere. In the reaction, two new carbon-carbon bonds were formed and one carbon-carbon bond was cleaved. It is very interesting to note that two different nucleophiles such as benzyl ketones and aromatics were coupled together without any metal which is unusual in organic synthesis (Figure b).

Publications

Total number of publications: 56**; Independent publications:** 24

Selected Publications

- Kishor P.; **Jeganmohan, M.**; "*ortho*-Benzoxylation of N-Alkyl Benzamides with Aromatic Acids Catalyzed by Ruthenium(II) Complex" *Chem. Eur. J.* **2014**, 20, 4092.
- Ravikiran CG; **Jeganmohan, M.**; "Ruthenium catalyzed *ortho*-arylation of acetanilides with aromatic boronic acids: an easy route to prepare phenanthridines and carbazoles" *Chem. Commun.*, **2014**, 50, 2442.
- Reddy, M. C.; **Jeganmohan, M.**; "Ruthenium-catalyzed cyclization of aromatic nitriles with alkenes: Stereoselective synthesis of (Z)-3-methyleneisoindolin-1-ones" *Org. Lett.*, **2014**, 16, 4866.
- More N. Y; **Jeganmohan, M.**; "Aerobic Dehydrogenative α-Diarylation of Benzyl Ketones with Aromatics through Carbon-Carbon Bond Cleavage" *Org. Lett.* **2014**, 16, 804.
- Manikandan R.; **Jeganmohan, M.**; "Ruthenium-Catalyzed Hydroarylation of Anilides with Alkynes: An Efficient Route to *Ortho*-Alkenylated Anilines" *Org. Lett.*, **2014**, 16, 912.

External Grants

- Total Synthesis of Natural Benzo[c]phenanthridine Alkaloids by Metal-Catalyzed Cyclization or C-H bond Activation reaction as a key step. Funding Agency: BRNS-DAE, India (Aug 2011-July 2014).
- Palladium-Catalyzed Chelation-Assisted C-H Bond Functionalization of Aromatics, Alkenes and Alkanes: SERB-DST, India (April 2012- March 2015).
- Ruthenium-Catalyzed Highly Regio-and Stereoselective Oxidative Coupling of π-Components: A Versatile Route to Substituted Alkenes, Dienes and Heterocycles: INSA, India (Oct 2014-Sept 2017).

Teaching Contributions

Organometallic Chemistry, Separation Principle and Techniques, Organic Synthesis I and II, Chemistry Lab II-Inorganic Chemistry, Advanced Organic Chemistry

Awards and Recognitions

- DAE Young Scientist Research Award, BRNS, BARC, 2011
- Young Associate, Indian Academy of Sciences, Bangalore, 2012-2015
- 2013: Science Academy Medal for Young Scientists, Indian National Science Academy, New Delhi
- 2013: Alkyl Amine-ICT young scientist award by Institute of Chemical Technology, Mumbai, India
- 2014: ISCB Award of Appreciation for Chemical Science

Research Group

Doctoral and project students: Kishor Padala, Ravi Kiran Chinnagolla, Mallu Chenna Reddy, Nagnath Yadav More, R. Manikandan, R. Manoharan, Sandeep Pimparker

Under-graduate students: M. Padmaja, Arjun Vijita

Past project student: D. Perumal

Past under-graduate students: Pilli Veena

ARNAB MUKHERJEE

Assistant Professor

Ph.D.: Indian Institute of Science, Bangalore, India
Post-doc.: EcoleNormaleSuperieure, Paris, France
Post-doc.: University of Colorado at Boulder, Colorado, USA
Joining at IISER: November 2009
Email: arnab.mukherjee@iiserpune.ac.in
URL: http://www.iiserpune.ac.in/~arnabm/

Computational Chemistry & Biophysics

The main research focus of this laboratory is to study molecular recognition processes (drug-DNA, protein-DNA) using computational methods (both classical and quantum). We calculate free energy profile for the recognition processes and from that probe into the detailed molecular mechanism.

DNA Intercalation is a method by which some anti-cancer drugs such as daunomycin, proflavine functions. Our study shows that the intercalation happens through a sequential process that defies natural fluctuation hypothesis and point towards a drug-induced cavity formation mechanism. We also showed the origin of experimentally observed millisecond timescale for the complex intercalation process of the proflavine molecule. Currently, we are working towards the dynamical effect of intercalation and protein-DNA interaction. Some of the results are shown in Fig. 1a.

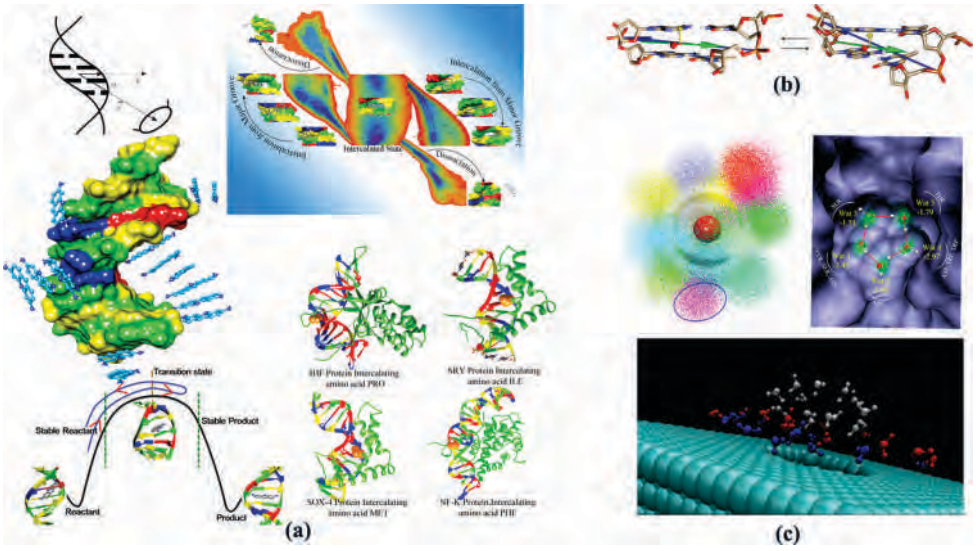


Figure 1: Representative image of (a) DNA Intercalation, (b) local conformational change in DNA, (c) the single water entropy.

Polymorphism of DNA is an interesting and fundamental biophysical phenomenon with a variety of biological implications. We have studied how, in the local dinucleotide level, the propensity of B- to A-form transition occurs in DNA (Fig. 1b). The ultimate goal of the study involved in structural transition of DNA is to find how this natural polymorphism can be used in nanodevices.

Design of a drug molecule often has a significant entropic contribution from water. Since slow water molecules contribute to free energetic stability upon replacement by a drug, it is important to identify the entropy of the individual water molecules. We developed a new method to calculate the entropy of a single water molecule and showed that in a single protein cavity, water molecules may have different entropy values (Fig. 1c). This method is being applied to calculate the single water entropy around DNA, around hydrophobic cavity.

Other studies involve protein misfolding, water residence time, azeotropic binary mixtures, etc.

Publications

Total number of publications: 30**; Independent publications:** 11

Selected Publications

- SahaT.; Dasari S.; Tewari, D.; Prathap A.; Sureshan, K. M.; Bera, A. K.; **Mukherjee, A.**;Talukdar, P. Hopping Mediated Anion Transport through a Mannitol-Based Rosette Ion Channel *J. Am. Chem. Soc.***2014**, *136*, 14128-14135..
- Kulkarni, **M.; Mukherjee, A.** Sequence Dependent Free Energy Profiles of Localized B- to A-Form Transition of DNA in Water *J. Chem. Phys.* **2013,** 139, 155102.
- Sasikala, W. D.; Mukherjee, A. Molecular Mechanism of Direct Proflavine-DNA Intercalation: Evidence for Drug-Induced Minimum Base-Stacking Penalty Pathway *J. Phys. Chem.* B **2012,** 116, 12208-12212.
- Wilhelm, **M.; Mukherjee, A.;** Bouvier, B.; Zakrzewska, K.; Hynes, J.T.; Lavery R. Multistep Intercalation Mechanism: Molecular Dynamics and Free Energy Studies of the Formation of a DNA-Daunomycin complex", *J. Am. Chem. Soc.* **2012,** 134, 8588-8596.
- **Mukherjee, A.** Entropy Balance in the Intercalation Process of an Anti-Cancer Drug Daunomycin *J. Phys. Chem. Lett.* **2011**, *2*, 3021-3026.

External Grants

- Dynamical Effects in the Mechanism of Intercalation of Anti-Cancer Drugs. Funding Agency: SERB-DST, India (May 2013-April 2016).

Teaching Contributions

Statistical Thermodynamics, Molecular Modeling and Simulation, Physical Chemistry Lab, General Chemistry

Research Group

Doctoral students: Wilbee D. Sasikala, Mandar Kulkarni, Sathish Dasari, Reman K. Singh, Debasis Saha

Int. Ph.D. students. Hridya V. M.

Past under-graduate students: Shreyas Supekar, Hutashan Vajpeyi

ANGSHUMAN NAG

Ramanujan Fellow

Ph.D.: Indian Institute of Science, Bangalore, India
Post-doc.: Indian Institute of Science, Bangalore, India
Post-doc.: University of Chicago, USA
Joining at IISER: November 2012
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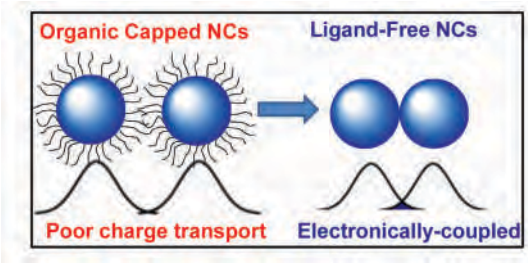
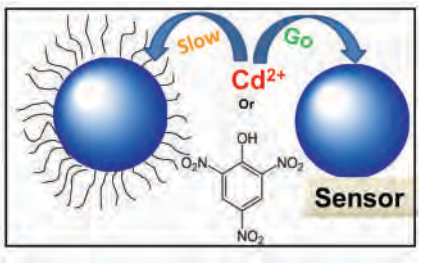
Colloidal Semiconductor Nanocrystals for Optoelectronics

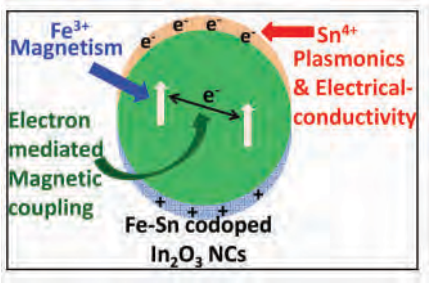
The main research focus of our group is on developing functional inorganic materials using solution processed semiconductor nanocrystal modules. The work can be divided into three major sections (i) material design mainly using colloidal organic-free nanocrystals, (ii) spectroscopic studies using luminescence and XAFS, and (iii) magneto- and opto- electronic applications forming flexible transparent conductor, solar cell and carrier mediated magnetic coupling.

Electronically Coupled All-Inorganic Nanocrystals (Surface Modification): Integration of nanocrystals in electronic and optoelectronic devices like photovoltaics, light-emitting-diodes (LEDs), photodetectors and printable electronics depends on the electronic property of the nanocrystal film, and thus on the interconnect between adjacent nanocrystals. However, colloidal nanocrystals are generally capped with an insulating organic layer. Consequently, the benefits of quantum confinement effect and solution processibility cannot be utilized because of inefficient injection or extraction of charge carriers. We are interested in designing organic-free semiconductor nanocrystals for various optoelectronic applications including solution processed transparent conductor and photovoltaics. Also, we employ such organic-free nanocrystals for chemical sensing simply because the fact that the analyte can interact easily with the bare nanocrystal surface, therefore, increasing sensitive.





Plasmonics, Electrical Conductivity, and Electron Mediated Magnetism from Doped Semiconductor Oxides. We are developing a unique category of material exhibiting the above mentioned three properties simultenously, via doping a magnetic ion in a transparent conducting oxide nanocrystal. For example, in Fe-Sn codoped In_2O_3 nanocrystals, localized surface plasmon resonance



band is observed in near to mid infrared region along with room temperature ferromagnetism and electrical conductivity >1 S/cm. More importantly, the electron mediated magnetic coupling can lead to spin based applications.

Publications

Total number of publications: 34**; Independent publications:** 7

Selected Publications

- Tandon, B.; Shanker, G. S.; **Nag, A.** Multifunctional Sn- and Fe-Codoped In_2O_3 Colloidal Nanocrystals: Plasmonics and Magnetism. *J. Phys. Chem. Lett.* **2014**, 5, 2306−2311.
- Swarnkar, A.; Shanker, G. S.; **Nag, A.** Organic-Free Colloidal Semiconductor Nanocrystals as Luminescent Sensors for Metal Ions and Nitroaromatic Explosives. *Chem Commun.* **2014**, 50, 4743-4746.
- Rao, M. J.; Shibata, T.; Chattopadhyay, S.; **Nag, A.** Origin of Photoluminescence and XAFS Study of $(ZnS)_{1-x}(AgInS_2)_x$ Nanocrystals**.** *J. Phys. Chem. Lett.* **2014**, 5, 167-173.
- Kadlag, K. P.; Patil, P.; Rao, M. J.; Datta, S.; **Nag, A.** Luminescence and Solar Cell from Ligand-Free Colloidal $AgInS_2$ Nanocrystals. *Cryst Eng Comm* **2014**, 16, 3605-3612.
- Kadlag, K. P.; Rao, M. J.; **Nag, A.** Ligand-Free, Colloidal, and Luminescent Metal Sulfide Nanocrystals. *J. Phys. Chem. Lett.* **2013**, 4, 167-1681.

External Grants

- Ligand-Free Colloidal All-Inorganic Semiconductor Nanocrystals: Synthesis, Photophysics and Optoelectronic Application. Funding Agency: SERB-DST, India (January 2014-January 2017).
- Optoelectronic and Plasmonic Properties of All-Inorganic Sn Doped In_2O_3 (ITO) Nanocrystal. Funding Agency: BRNS-DAE, India (July 2013- July 2017)**.**
- DST-SERB Ramanujan Fellow Research Grant (November 2012-November 2017).

Teaching Contributions

Solid State Chemistry, Physical Chemistry of Solutions, Chemistry Lab II-Inorganic Chemistry, Advanced Inorganic Laboratory

Awards and Recognitions

- National Academy of Science India (NASI)-Young Scientist Platinum Jubilee Award 2014
- Associate of the Indian Academy of Sciences Bangalore 2014
- Toulouse medal for the best Ph. D. thesis in SSCU by IISc Bangalore, 2009

Research Group

Doctoral and project students: Abhishek Swarnkar, Bharat Tandon, G. Shiva Shanker, Kadlag Kiran Parashram, Metikoti Jagadeeswara Rao, Naziya Paeveen, Wasim Jeelani Mir

Under-graduate students: Aditya Katti, Aswathi Ashok, Bala Gopal M, Sreejith P Nandan

PRAMOD P. PILLAI

Assistant Professor

Ph.D.: National Institute for Interdisciplinary Science and Technology (NIIST), Trivandrum, India
Post-doc.: Technische Universität Dortmund, Germany
Post-doc.: Northwestern University, Illinois, USA
Joining at IISER: June 2014
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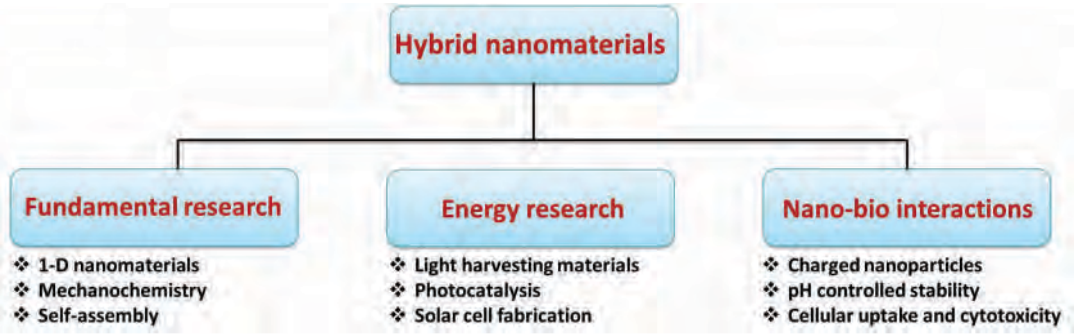
Functional Nanomaterials: From Photochemistry to Biotargeting

The main research focus of this laboratory is on the design and synthesis of hybrid nanostructures for fundamental as well as applied studies. The research involves various techniques in nanoscience and nanotechnology to address two global concerns: (1) energy and (2) therapeutics.



Fundamental research: Integration of nanomaterials into higher order nanostructures results in new and advanced properties that are absent at the individual level. The main aim here is to develop simple and robust synthetic strategies through which the interaction between individual nanoparticles can be controlled in a precise manner. The well-ordered nanoparticle suprastructures formed as a result of these controlled interactions will be used for sensing and electrical studies. Emphasis is also given for developing new materials platform for studying the electron transport and mechanical properties at the nanoscale.

Energy research: The ultimate aim here is to improve the stability of the charge separated species in a light harvesting material, and thereby improve its overall efficiency. Efforts are to develop heterostructures based on metal and semiconductor nanomaterials for studying the effect of geometries, compositions and configurations on the stability of photogenerated electron-hole pairs. The inclusion of metal nanostructures, as one of the components, is expected to enhance the overall efficiency of the photovoltaic device due to its (i) electron storage/transport capability and (ii) light concentration property through a strong near-field enhancement by the surface plasmon effect.

Nano-bio interactions: The focus is on providing insights into the basic question - how to improve the stability and specific targeting of NPs in biological studies. Many factors such as size, shape and surface chemistry, decide the fate of the interactions between NPs and biosystems. Among them, the surface chemistry (charge, functionality, ligand arrangement, hydrophobicity and hydrophilicity) plays a crucial role. Here, the emphasis is on tuning the surface properties of metal/semiconductor NPs by incorporating both ionizable (to achieve variable surface charge) and biotargeting groups, simultaneously. These multifunctional NPs is expected to exhibit advanced biophysical properties such as improved biostability and circulation time, controlled cellular uptake, reduced non-specific binding etc.

Publications

Total number of publications: 13

Selected Publications

- Demirörs. A. F.; **Pillai, P. P.;** Kowalczyk, B.; Grzybowski, B. A. "Colloidal Assembly Directed by Virtual Magnetic Moulds" *Nature* **2013**, *503*, 99 - 103.
- **Pillai, P. P.;** Huda, S.; Kowalczyk, B.; Grzybowski, B. A. "Controlled pH Stability and Adjustable Cellular Uptake of Mixed-Charge Nanoparticles" *J. Am. Chem. Soc.* **2013**, *135,* 6392 - 6395.
- Pillai, P. P.; Pacławski, K.; Kim, J.; Grzybowski, B. A. "Nanostructural Anisotropy Underlies Anisotropic Electrical Bistability" *Adv. Mater.* **2013**, *25,* 1623 - 1628.
- **Pramod, P.**; Thomas, K. G. "Plasmon Coupling in Dimers of Au Nanorods" *Adv. Mater.* **2008**, *20,* 4300 – 4305.
- **Pramod, P.**; Joseph, S. T. S.; Thomas, K. G. "Preferential End Functionalization of Au nanorods Through Electrostatic Interactions" *J. Am. Chem. Soc.* **2007**, *129,* 6712 - 6713.

External Grants

- Curvature Controlled Chemical Reactivity and Location Specific Assembly of Nanoparticles. Funding Agency: BRNS-DAE, India. *(Submitted).*

Teaching Contributions

Fundamentals of Molecular Spectroscopy, Chemistry Laboratory I - Physical Chemistry

Awards and Recognitions

- Alexander von Humboldt Fellow

Research Group

Project student: Sumit Bhosale

MRINALINI PURANIK

Associate Professor

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Post-doc.: Princeton University, USA
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Biomolecular Structure and Dynamics

Current interests:

- Understanding the role of fast, local residue motion in enzyme catalysis
- Structure-function relationships in enzymes to understand interactions with small molecules, folding and aggregation in proteins[1]
- Recognition and repair of damaged DNA by enzymes to understand mechanisms of drug resistance
- Excited state dynamics, intramolecular relaxation and reactivity of nucleic acids[4], aminoacids[2,3] and flavins
- Structure and organization of melanin pigment in mammals, understanding polymerization and aggregation processes

Excited state dynamics of nucleobases and nucleic acids: DNA Nucleobases have fascinating, unusual photophysics. They have extraordinarily short-lived excited states (~500fs - few ps) that provide stability under ultraviolet radiation making them ideal carriers of genetic information. While the four common nucleobases have been extensively studied, very little is known of other biologically important nucleobases. I am interested in understanding: the relationship between structure and photophysics of nucleobases, the mechanisms of relaxation upon photoexcitation, and reorganization of inter- and intra-molecular coupling with different excocyclic substitutions, protein and solvent environments. We have made extensive ultraviolet resonance Raman measurements and computational calculations of ground and excited state structures and dynamics of nucleobases. We have established their solution structures, vibrational signatures, protonation states and made quantitative measurements of Raman intensity profiles. We are now using wave packet dynamical modeling in conjunction with experimental and ab initio data to determine excited state structure and delineate homogeneous and inhomogeneous contributions at <100 fs.

Role of fast local motion in enzyme catalysis: My goal is to measure the femtosecond dynamics of nucleobases, aminoacids and proteins in three contexts. With a small protein, Barstar we have measured the timescale and magnitude of residue dynamics in the core of natively folded protein.[3,4] Increasing the complexity of the system, we next wish to understand to measure femtosecond dynamical coupling between a nucleotide substrate and an enzyme, human HGPRT, a ribosyl transferase. We wish to understand the role of the fast, local motions in assisting the chemical step of conversion of substrates to products.

Structure and organization of the melanin pigment: Melanin is one of the least understood biopolymers. Its unusual properties – optical opacity, heterogeneity and insolubility make it a challenging

system to work with. We are using a host of biophysical techniques and computational modeling to develop fundamental understanding of the structure and organization of the melanin pigment in isolation and within intact human cells.

Publications

Total number of publications: 23**; Independent publications:** 11

Selected Publications

- Karnawat, V.; Balaram, H. and **Puranik, M.** Differential distortion of purine substrates by human and Plamodium falciparum HGPRT to catalyze formation of mononucleotides, *J. Phys. Chem.* **2015,** in press.
- Ramachandran, G.; Milán-Garcés, E.; Udgaonkar, J. B. and **Puranik, M.** Resonance Raman spectroscopic characterization of the kinetics of tau fibril formation, *Biochemistry* **2014,** *53*, 6550-6565.
- Milan-Garcés, E.; Udgaonkar, J. B.; and **Puranik, M.** Intricate packing in the hydrophobic core of barstar through a 'CH-pi' interaction', *Journal of Raman Spectroscopy* **2014,** *45*, 814-821.
- Milan-Garcés, E.; Kaptan, S. and **Puranik, M.** Mode-specific reorganization energies and ultrafast solvation dynamics of Tryptophan from Raman line-shape analysis, *Biophysical Journal* **2013**,*105*, 211-221.
- Gogia, S. and **Puranik, M.** Solution structures of purine base analogues 6-chloroguanine, 8-azaguanine and allopurinol, *Journal of Biomolecular Structure and Dynamics* **2014,** *32*, 27-35.

External Grants

- Biophysical studies of structure and organization of human pigment melanin, Program Grant, DBT, India
- Mechanisms of recognition and repair of unwanted methylation on DNA by the repair enzyme AlkB**,** DBT, India
- Recognition and repair of oxidative damage in DNA by Formamidopyrimidine DNA glycosylase, DBT, India

Teaching Contributions

Thermodynamics, Fundamentals of Molecular Spectroscopy, Advanced Molecular Spectroscopy, Physical Chemistry Laboratory

Awards and Recognitions

- Innovative Young Biologist Award, DBT, India
- Max-Planck India Fellow

Research Group

Doctoral and project students: Sayan Mondal, Vishakha Karnawat, Sudeb Ghosh, Yashwant Kumar, Anil Yadav, Shahila Mohammed, Prashant Badgujar

Under-graduate students: Arya Thampi, Siddhartha Sohoni

Past doctoral students: Dr. Spriha Gogia, Dr. Namrata Jayanth, Dr. Erix Milan-Garces

Past under-graduate students: Abhishek Kumar, Sagar Gore, Varun Kumar

BRITTO S. SANDANARAJ

Assistant Professor

Ph.D.: University of Massachusetts - Amherst, USA
Post-doc.: Novartis Institutes for Biomedical Research (NIBR), Inc - Boston & The Scripps Research Institute, California, USA
Previous position: Senior Scientist, RNAi Therapeutics, NIBR, Boston, USA
Joining at IISER: February 2014
Email: sandnaraj.britto@iiserpune.ac.in
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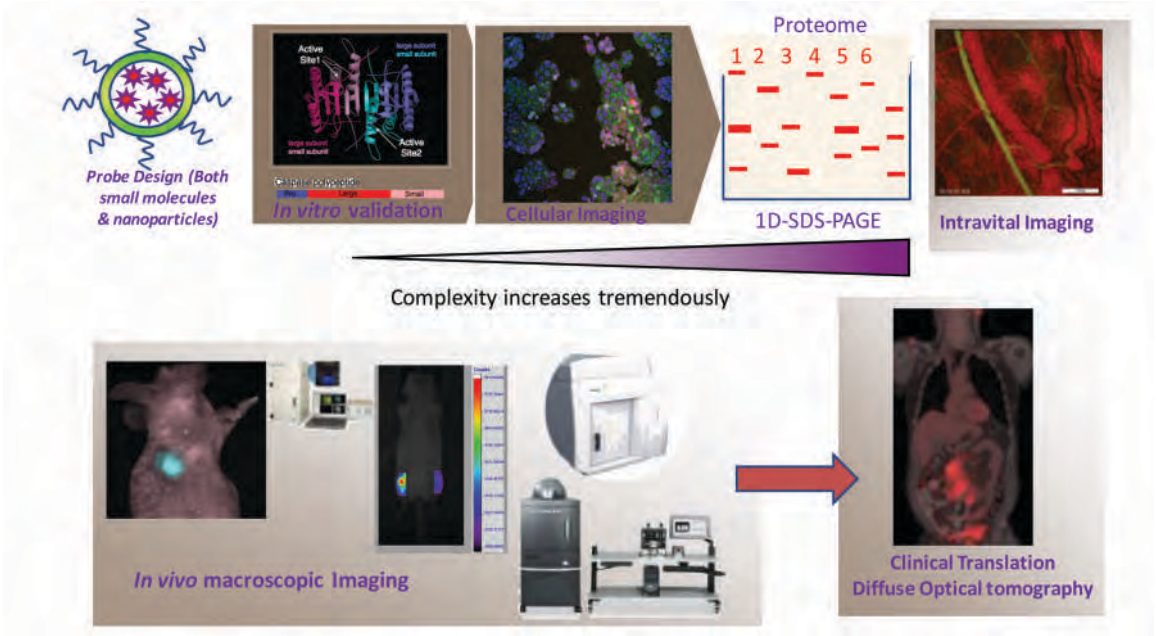
Chemical Biology/Physiology & Optical Molecular Imaging

Developing New Technologies for Accurate and Specific Detection of "Active Enzymes" In Vivo Study of enzyme function at single molecule resolution with very high substrate specificity is still a technical challenge. We have been interested in study of purified enzymes and cell/tissue lysates to monitor their active function in native conditions in the milieu of all other components of living cells, with very high resolution and exquisite specificity. Such studies will help understand the precise chemistry behind enzyme-substrate interactions and in regulation of complex biochemical reactions under various conditions. We are developing technology to study enzyme function *in vivo* at very high temporal resolution and substrate specificity with application to understand diseases and test the efficiency of targeted drugs. Major effort of our research is the design and synthesis of chemical reporters (both small molecule & macromolecule) to probe the function of particular enzyme function *in vivo*. The synthesized probes will be validated at different levels starting from testing with purified enzymes, cellular validation, *in vivo* and *ex vivo* validation. This kind of bottom-up approach is must for accurate and specific detection of active enzymes *in vivo*.



Publications

Total number of publications: 14

Selected Publications

- Krucker, T.; **Sandanaraj, B. S.;** Spelling Optical Imaging for New Grammar of Drug Discovery *Phil. Trans. Royal Soc. London. A* **2011**, *369*, 4651-4665
- **Sandanaraj, B. S.**; Kneuer, R.; Beckmann, N. Optical and Magnetic Resonance Imaging as Complementary Modalities in Drug Discovery *Future Med Chem* **2010**, *3*, 317-337
- **Sandanaraj, B. S.;** Gremlich, H-U.; Kneuer, R.; Dawson, J.; Wacha, S. Fluorescent Nanoprobes as a Biomarker for Increased Vascular Permeability: Implications in Diagnosis and Treatment of Cancer and Inflammation *Bioconju. Chem.* **2010**, *21*, 93-101
- **Sandanaraj, B. S.**; Demont, R.; Thayumanavan, S. Generating Patterns for Sensing Using a Single Receptor Scaffold *J. Am. Chem. Soc.* **2007**, *129*, 3506-3507
- **Sandanaraj, B. S.**; Demont, R.; Aathimanikandan, S. V.; Savariar, E. N.; Thayumanavan, S. Selective Sensing of Metalloproteins from Non-selective Binding using a Fluorogenic Amphiphilic Polymer *J. Am. Chem. Soc.* **2006**, *128*, 10686-10687
- **Sandanaraj, B. S.**; Vutukuri, D. R.; Simard, J. M.; Klaikherd, A.; Hong, R.; Rotello, V. M.; Thayumanvan, S. Noncovalent Modification of Chymotrypsin Surface Using an Amphiphilic Polymer Scaffold : Implications in Modulating Protein Function *J. Am. Chem. Soc.* **2005**, *127*, 10693-10698
- Basu, S.; Vutukuri, D. R.; Shyamroy, S.; **Sandanaraj, B. S.**; Thayumanavan, S. Invertible Amphiphilic Homopolymers *J. Am. Chem. Soc.* **2004**, *126*, 9890-9891

Teaching Contributions

Chemical Biology, Organic Chemistry lab.

Research Group

Doctoral and Project Students: Mohan Kumar Reddy, Pavan Kumar Bhandari

Project Students: Santosh Surve, Ananth Kumar

Under-graduate Students: Jocinth Selvakumar

SEERGAZHI G. SRIVATSAN

Associate Professor

Ph.D.: Indian Institute of Technology, Kanpur, India
Post-doc.: Alexander von Humboldt Fellow, University of Bonn, Germany
Post-doc.: University of California, San Diego, USA
Assistant Professor: November 2008 – December 2014, IISER-Pune
Associate Professor: December 2014 – Present date, IISER-Pune
Email: srivatsan@iiserpune.ac.in
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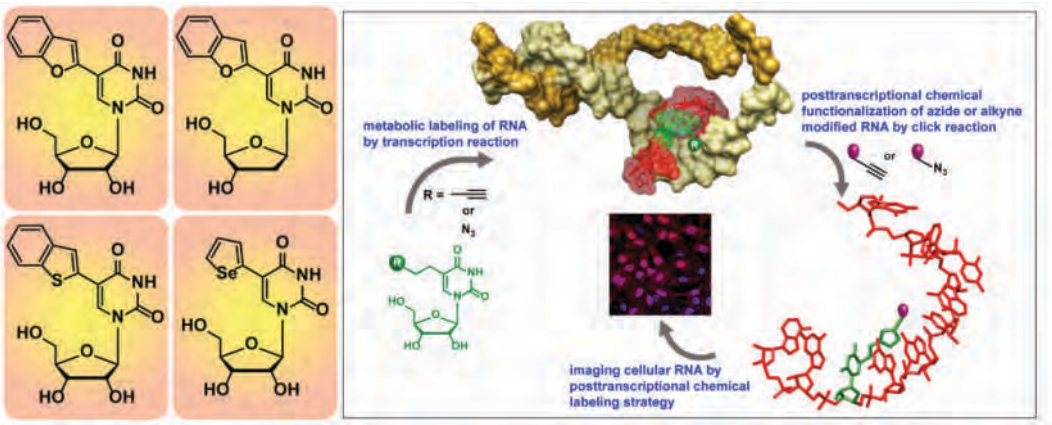
Chemical Biology: Nucleic Acid Chemistry and Biophysics

My group is interested in developing tools to assess biological events by utilizing contemporary nucleic acid functions and synthetic biology. In particular, we are interested in developing biophysical tools that would enable the study of nucleic acid structure, dynamics and function in vitro and in cells. We are also interested in developing multifunctional nucleolipid conjugates that could self-assemble into nanofibres, nanotubes and gels. We expect that these self-assemblies would provide platforms for designing biosensors, biomaterials and scaffolds for nontemplate oligomerization of nucleic acids.

Functionalized nucleoside analogues: We have initiated a research program to develop structurally non-perturbing and conformation-sensitive fluorescent nucleoside analogue probes for studying nucleic acid structure, dynamics and recognition properties. Some of the analogues, which we have developed, are highly sensitive to conformational changes. We have utilized them in developing fluorescence assays to (i) detect abasic sites (depurinated site) in DNA and RNA, (ii) monitor RNA-drug binding and (iii) study oligonucleotide dynamics in cell-like confined environment. Currently, we are developing multifunction nucleoside probes, which could be used to study the structure and function of nucleic acid simultaneously by fluorescence and NMR spectroscopy and by X-ray crystallography.

Chemical labeling and imaging of RNA: We have developed a practical chemical labeling and imaging technique for cellular RNA by using novel toolbox made of azide- and alkyne-modified UTP analogues. These analogues are readily incorporated into transcribing RNA by endogenous RNA polymerases, which can be posttranscriptionally labeled with a variety of probes by bioorthogonal reactions such as click and Staudinger ligation reactions.



Publications

Total number of publications: 42**; Independent publications:** 15

Selected Publications

- Sabale, P. M.; George, J. T.; **Srivatsan, S. G.** Base-modified PNA-graphene oxide platform as a turn-on fluorescence sensor for the detection of human telomeric repeats. *Nanoscale* **2014**, *6*, 10460-10469.
- Tanpure, A. A.; **Srivatsan, S. G.** Synthesis, photophysical properties and incorporation of a highly emissive and environment-sensitive uridine analogue based on the lucifer chromophore. *ChemBioChem* **2014**, *15*, 1309-1316.
- Rao, H.; Sawant, A. A.; Tanpure A. A.; **Srivatsan, S. G.** Posttranscriptional chemical functionalization of azide-modified oligoribonucleotides by bioorthogonal click and Staudinger reactions, *Chem. Commun.* **2012**, *48*, 498–500.
- Rao, H.; Tanpure A. A.; Sawant, A. A.; **Srivatsan, S. G.** Enzymatic incorporation of an azide-modified UTP analog into oligoribonucleotides for post-transcriptional chemical functionalization. *Nature Protocols* **2012**, *7,* 1097–1112.
- Pawar, M. G.; **Srivatsan, S. G.** Synthesis, photophysical characterization, and enzymatic incorpora-tion of a microenvironment-sensitive fluorescent uridine analog. *Org. Lett.* **2011**, *13*, 1114–1117.

External Grants

- Fluorescent Nucleoside-Based Amphiphiles: Synthesis, Self-Assembly Properties and Applications. Funding Agency: CSIR, India (November 2012-November 2015).
- Equipment grant. Funding Agency: Alexander von Humboldt Foundation, Germany.
- Functionalized Ribonucleoside Analogues: Synthesis, Site-Specific Enzymatic Incorporation and Applications. Funding Agency: SERB-DST, India (April 2010-March 2013).

Teaching Contributions

General Chemistry, Bioorganic Chemistry, Chemical Biology, Structural Methods and Analysis, Chemistry Lab I-Phy. Chem., Chemistry Lab III-Org. Chem. and Advanced Organic Chemistry Lab

Awards and Recognitions

- Emerging young scientist in India: awarded at the Chemical Frontiers Conference 2014
- RSC West India Section: Early Career Scientist award 2012
- IUPAC Prize for Young Chemists, 2004

Research Group

Doctoral students: Maroti Pawar, Anupam Sawant, Arun Tanpure, Pramod Sabale, Ashok Nuthanakanti, Sudeshna Manna, Jerrin Thomas George, Manisha Walunj

Undergraduate students: Sarangamath Sangamesh

Past undergraduate students and project fellows: Haritha Rao, Anurag Agrawal, Pooja Patheja, Progya Mukherjee, Shewta Yelgaonkar, Siddheshwar Aland

PINAKI TALUKDAR

Assistant Professor

Ph.D.: University of Geneva, Switzerland
Post-doc.: University of Illinois, Urbana-Champaign, USA
Previous positions: Senior Research Scientist, AMRI Global Inc., India
Senior Research Scientist, ILS, Hyderabad
Joining at IISER: July 2009
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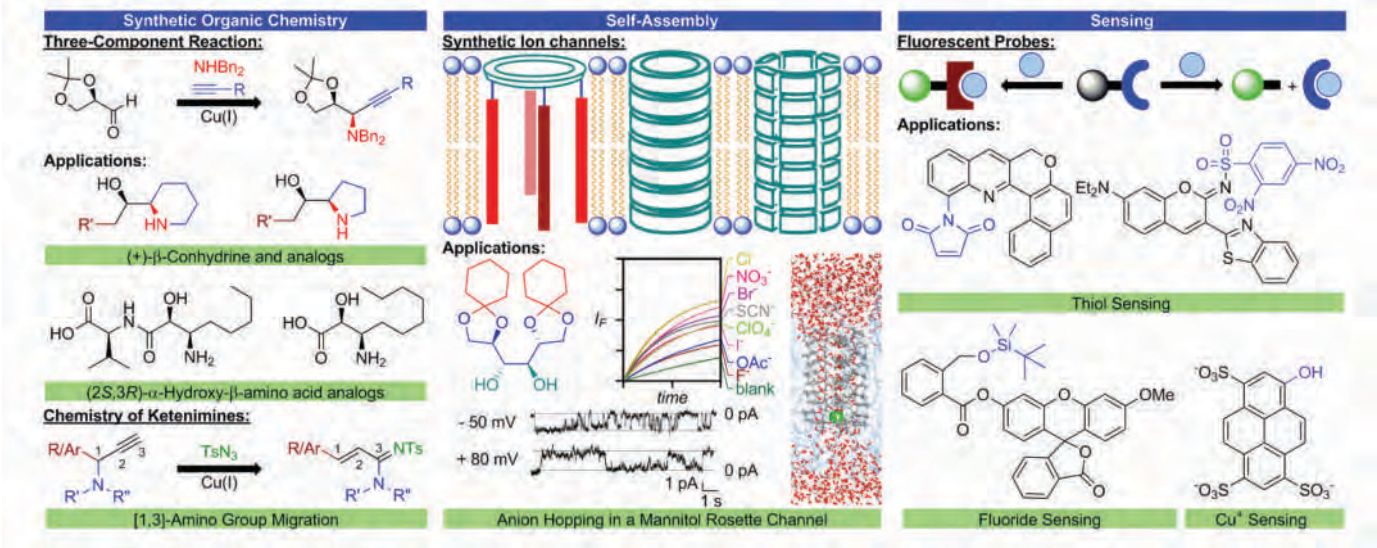
Synthesis, Self-Assembly and Sensing

The main research focus of this laboratory is to combine the knowledge of organic synthesis and supramolecular interactions to design molecules for functional applications.

Targeted synthesis of molecules is essential in total synthesis, medicinal chemistry, chemical biology, supramolecular chemistry, etc. We have established Cu(I) catalyzed aldehyde-amine-alkyne coupling reaction as an efficient methodology for the construction of (2*S*,3*R*)-α-amino alcohol derivatives. The methodology was applied further in the synthesis of various natural products. We have also developed [1,3]-amino group migration strategy for the synthesis of acrylamidines.

Self-assembly of molecules plays crucial roles in diverse physical, chemical and biological phenomena. Our interest is to design artificial supramolecular ion channels and pores, and mimic the functions their natural siblings. We have constructed unimolecular ion channels based on cyclo-oligo-glucosamines for tuning of ion transport activity. We have also reported mannitol based rosette ion channels. These channels allow selective anion transport via a hopping mechanism of ion from one rosette to the next.



Sensing of species that are of either biological or environmental interests, is essential for understanding their functions and effects. Our laboratory has developed large number of fluorescent probes for the

sensing of thiols (*e.g.* biothols, aryl thiols, H_2S), anions (*e.g.* fluoride ion), cations (*e.g.* cations), etc. These probes are useful for rapid, selective and sensitive detection of respective analytes, and applicable for live cell imaging studies.

Publications

Total number of publications: 36 **Independent publications:** 23

Selected Publications

- Deshmukh, S. C.; **Talukdar, P**. Stereoselective synthesis of (2S,3R)-α-hydroxy-β-amino acids (AHBAs): valinoctin A, (2S,3R)-3-amino-2-hydroxydecanoic acid and a fluorescent-labeled (2S,3R)-AHBA. *J. Org. Chem.* **2014**, DOI: 10.1021/jo501751u.
- Saha, T.; Dasari, S.; Tewari, D.; Prathap, A.; Sureshan, K. M.; Bera, A. K.;* Mukherjee, A.; **Talukdar, P.** Hopping-mediated anion transport through a mannitol-based rosette ion channel. *J. Am. Chem. Soc.* **2014**, 136, 14128-14135.
- Saha, T.; Roy, A.; Gening, M. L.; Titov, D. V.; Gerbst, A. G.; Tsvetkov, Y. E.; Nifantiev, N. E.; **Talukdar, P.** Cyclo-oligo-(1→ 6)-β-D-glucosamine based artificial channels for tunable transmembrane ion transport. *Chem. Commun.* **2014**, 50, 5514-5516.
- Roy, A.; Kand, D.; Saha, T.; **Talukdar, P.** A cascade reaction based fluorescent probe for rapid and selective fluoride ion detection. *Chem. Commun.* **2014**, 50, 5510-5513.
- Chauhan, D. P.; Varma, S. J.; Vijeta, A.; Banerjee, P.; **Talukdar, P.** A 1,3-amino group migration route to form acrylamidines. *Chem. Commun.* **2014**, 50, 323-325.

External Grants

- Studies on non-covalent modulation of gating and selectivity of synthetic ion channels. Funding Agency: SERB-DST, India (May 2013 – April 2016).
- Study of transmembrane ion channel activity of cyclo-(1→ 6)-β-D-glucosamine derivatives and evaluation of their antibacterial potential. Funding Agency: DST, India under DST-RFBR scheme (Sep, 2011 – Sept 2013).

Teaching Contributions

Self-assembly in chemistry, Structural methods and analysis, Physical organic chemistry, Introductory chemistry III-Organic chemistry, Organic chemistry laboratory courses, Lab training/theory projects

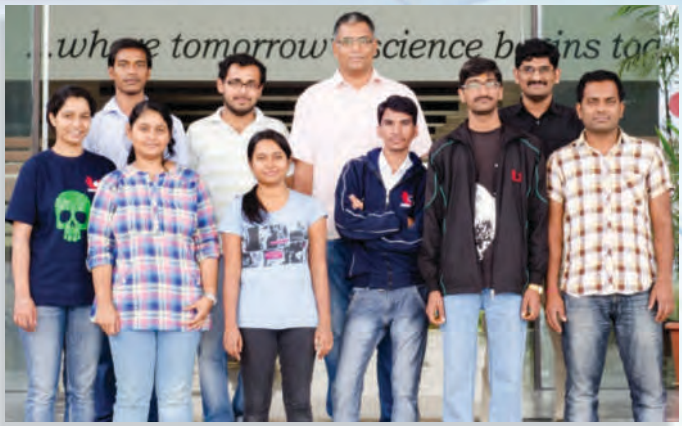
Research Group

Doctoral and project students: Dnyaneshwar Kand, Sharad Chandrakant Deshmukh, Dinesh Pratapsinh Chauhan, Tanmoy Saha, Arundhati Roy, Sopan Shinde, Sanjit Dey, Manjit Kaur

Under-graduate students: Pratyush K. Mishra, Shivgan Aishwary Tukaram, Konoya Das

Past doctoral students: Dnyaneshwar Kand

Past under-graduate students: Ashutosh Priyadarshi, Sreejith J. Varma



R. VAIDHYANATHAN

Assistant Professor

Ph.D.: JNCASR, Bangalore, India
Post-doc.: University of Liverpool, UK
Post-doc.: University of Calgary, Canada
Joining at IISER: February 2012
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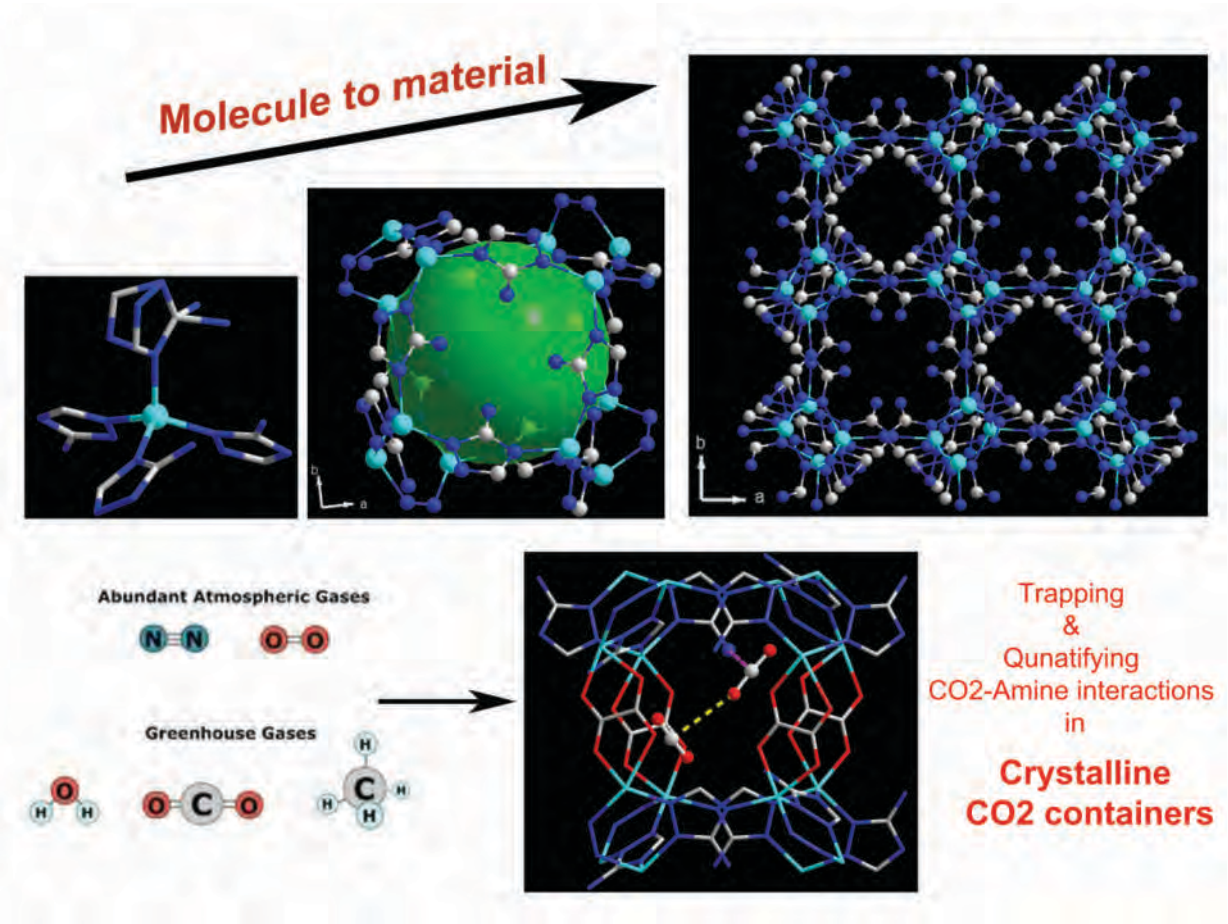
URL: http://www.iiserpune.ac.in/~vaidhya/

Advanced Porous Materials Chemistry

The main research focus of this laboratory is on designing and developing porous solids for application in CO_2 capture and in capture and separation of other industrially valuable gases. The chemistry includes the functionalization of the surfaces of the pores with gas specific functionalities. The materials generated as crystals or crystalline powders are characterized using SXRD, PXRD, SEM, TEM etc. We also use powder based structural solution techniques such as Reitveld, Pawley routines.



Other areas of interest pertain to developing chiral solids for heterogeneous enantio-separation and catalysis. We develop hierarchy of inorganic-organic solids capable of exhibiting properties ranging from insulating to semi conducting to conducting. Such solids would be engineered for their potential application in fuel cells, solar cells and other areas of alternate energy.

Publications

Total number of publications: 40**; Independent publications:** 2

Selected Publications

- Shyamapada Nandi and **Ramanathan Vaidhyanathan**. *J. Chem. Sci.* **2014**, *126*, 1393–1398.
- **Ramanathan Vaidhyanathan**, Metal Organic Framework – Crystalline stacked molecular containers, *Resonance* (in press, **2014**).
- **Ramanathan Vaidhyanathan**, Simon S. Iremonger, George K. H. Shimizu, Peter G. Boyd, Saman Alavi, Tom K. Woo, Competition and Cooperativity in Carbon Dioxide Sorption by Amine-Functionalized Metal–Organic Frameworks. *Angew. Chem. Int. Ed.* **2012**, *51,* 1826 –1829.
- **Ramanathan Vaidhyanathan**, Simon S. Iremonger and Peter Boyd, Saman Alavi, Tom K. Woo, George K. H. Shimizu. Direct observation and quantification of CO_2 binding within amine-functionalized nanoporous solids. *Science,* **2010**, *330*, 650.

External Grants

- Industrial Grant via a MoU between Enovex, Canada and IISER Pune, (May 2012-present).
- Centre for Excellence in Energy. Funding Agency: MHRD, India (October 2014).

Teaching Contributions

Inorganic chemistry to freshmen and Advanced Materials Chemistry for graduate students

Research Group

Doctoral students: Shyamapada Nandi (Prime Minister Fellow), Shalini, Aparna Banerjee (Prime Minister Fellow), Dinesh Mullangi

Under-graduate students: Bhavin Choksi and Nidhi Sudhir

ARUN VENKATNATHAN

Associate Professor

Ph.D.: Indian Institute of Technology, Bombay, India
Post-doc.: UCLA, University of Utah, Pacific Northwest National Laboratory
Assistant Professor: July 2008 – December 2014, IISER-Pune
Associate Professor: December 2014 – Present date, IISER-Pune
Email: arun@iiserpune.ac.in
URL: http://www.iiserpune.ac.in/~arun/

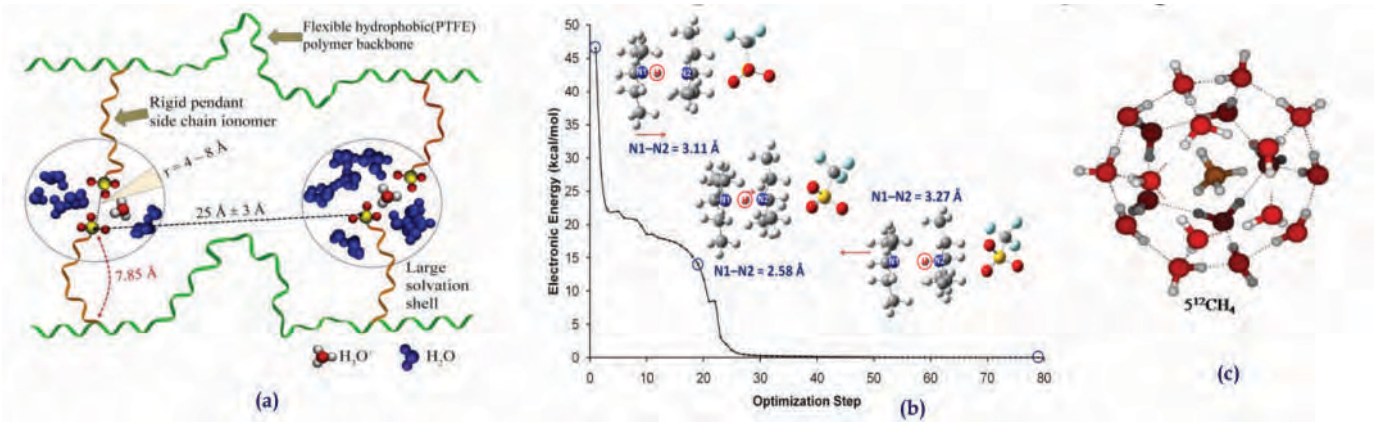
Computational Chemistry of Materials for Energy

The main research focus of this laboratory lies in the application of quantum chemistry methods, force-field development and application of Molecular Dynamics simulations to characterize molecular and nano-scale properties of soft materials of relevance to energy storage and conversion.

Force-Fields are developed for Triflic acid fragments as Proton Conducting Groups of Polymer Electrolyte Membranes (PEM). Molecular Dynamics (MD) simulations are used for characterization of structural properties (Radial Distribution Functions, see schematic Figure a) of Perfluorosulfonic Acid and Benz-imidazole based PEMs and molecular transport under various fuel cell operating conditions.

Mechanism of Proton Transport in Ionic Liquid Doped Membranes is investigated (Figure b) using Gas-Phase Quantum Chemistry Calculations. Structure and Dynamics of hydrated Imidazolium Ionic Liquids is also characterized using MD simulations.

Density Functional Theory (with dispersion included functionals) accurately predict spectral properties of occupancy of methane and hydrogen in cages (Figure c) of clathrate hydrates and supports Raman spectroscopy experiments.



Publications

Total number of publications: 33**; Independent publications:** 18

Selected Publications

- Ramya, K. R.; Kumar, P.; Kumar, A.; **Venkatnathan, A.** Interplay of Phase Separation, Tail Aggregation, and Micelle Formation in the Nanostructured Organization of Hydrated Imidazolium Ionic Liquid. *J. Phys. Chem. B* **2014**, 118, 8839.
- Kumar M.; **Venkatnathan, A.** Mechanism of proton transport in ionic liquid doped Perfluorosulfonic acid membranes. *J. Phys. Chem. B* **2013**, 117, 14449.
- Sunda, A. P.; More M.; **Venkatnathan, A.** A Molecular investigation of nanostructure and dynamics of Phosphoric/Triflic acid blends of hydrated ABPBI [poly(2,5-benzimidazole)] Polymer Electrolyte Membrane. *Soft Matter.* **2013**, 9 (4), 1122.
- Sunda, A. P.; **Venkatnathan, A.** Molecular Dynamics Simulations of Side Chain Pendant of Perfluorosulfonic Acid Polymer Electrolyte Membranes. *J. Mater. Chem. A.* 2013, 1 (3), 557.
- Ramya, K. R.; Pavan Kumar G. V.; **Venkatnathan, A.** Raman spectra of vibrational and librational modes of methane clathrate hydrates using Density Functional Theory. *J. Chem. Phys.* 2012, 136, 174305.

External Grants

- Molecular modeling and simulation of nanostructure and dynamics of ionic liquid doped polymer electrolyte membrane fuel cells, Funding Agency: SERB-DST, India (August 2013-August 2016).
- Modeling and simulation of polymer electrolyte membranes and molecular transport in fuel cells, Funding Agency: SERB-DST, India (March 2010- March 2013).

Teaching Contributions

Introductory Physical Chemistry, Quantum Chemistry, Advanced Physical Chemistry Laboratory, Molecular Modeling and Simulation

Research Group

Doctoral and project students: Minal More, Praveen Kumar, Rakesh Pant, Prabhat Prakash

Under-graduate student: Sourabh

Past Postdoc: Dr. Milan Kumar (Faculty at RGIPT)

Past doctoral students: Dr. Anurag Sunda (JNCASR, Bengaluru), Dr. K. R. Ramya (University of Iceland)

Past under-graduate student: Rohit Kumar

O. T. MUHAMMED MUSTHAFA

Assistant Professor

Ph.D.: Indian Institute of Science, Bangalore, India
Post-doc.: University of St-Andrews, Scotland, UK
Post-doc.: Indian Institute of Science, Bangalore, India
Collaborative Researcher: Université Joseph Fourier - Grenoble, France
Joining at IISER: August 2014
Email: musthafa@iiserpune.ac.in
URL: http://www.iiserpune.ac.in/~musthafa/

Electrochemistry, Energy Storage and Conversion

The main research focus of our energy laboratory is understanding the complex phenomena at the electrode/electrolyte interface by a range of electrochemical, microscopic and spectroscopic techniques and extending the fundamental understanding we gain at the molecular level to design cost effective, economical and environmentally friendly energy storage and conversion devices. Further in a different perspective we are evangelistic in exploring new horizons in electrochemistry for developing novel interfaces for applications ranging from selective sensors to electro-organic synthesis. My main research areas are: Interfacial Electrochemistry, Fuel cells, Supercapacitors, Batteries and Sensors.

Publications

Total number of publications: 10

Selected Publications

- **Muhammed M. Ottakam Thotiyl.;** Freunberger, S.; Peng, Z.; Chen, Y.; Liu, Z.; Peter G Bruce. A stable cathode for aprotic Li-O_2 battery. *Nature Materials* **2013,** *12,* 1050-1056.
- **Muhammed M Ottakam Thotiyl.;** Freunberger, S.; Zhanquan Peng.; Peter Bruce. The carbon electrode in Non-aqueous Li-O_2 cells. *J. Am. Chem. Soc.* **2013,** *135,* 494-500.
- **Muhammed. M. Ottakam Thotiyl.;** Basit, H.; Sanchez, J. A.; Goyer, C.; Guerente, L. C.; Dumy, P.; Sampath, S.; Labbe, P.; Moutet, J. C. Multilayer assemblies of polyelectrolyte-gold nanoparticles for the electrocatalytic oxidation and trace detection of arsenic (III). *J. Colloid and Interface Science,* **2012,** *383,* 130-139.
- **Muhammed. M. Ottakam Thotiyl.;** Kumar, T. R.; Sampath. S. Pd supported on titanium nitride for efficient ethanol oxidation. *J. Phys. Chem. C,* **2010**, *114,* 17934–17941.
- **Muahmmed Musthafa O. T.**; Sampath, S. High performance platinized titanium nitride catalyst for methanol oxidation. *Chem. Commun.,* **2008**, 67-69.

External Grants

- Rechargeable CO_2 /O_2 electrode for air breathing Energy Storage Devices. Funding Agency: SERB-DST, India. Submitted.
- Engineering the Carbon Surface while Preserving its Inherent Physicochemical Characteristics: Towards nanoscale modification of carbon electrode for Rechargeable Batteries and Fuel cells**:** DAE, India. Submitted.

Awards and Recognitions

- Rhone-Alps research fellowship-French Embassy-2009
- EPSRC research fellowship-UK-2011

MOUMITA MAJUMDAR

Assistant Professor

Ph.D.: Indian Institute of Technology, Kanpur, India
Post-doc.: Osaka University, Japan (Specially Appointed Assistant Professor)
Post-doc.: Saarland University, Germany
Joining at IISER: October 2014
Email: moumitam@iiserpune.ac.in
URL: http://www.iiserpune.ac.in/people/faculty-details/142

Main Group Chemistry-Catalysis and Materials Applications

Our research focus is to expand the chemical functionalities of low-valent compounds spanning the Groups 13-15 of the periodic table. Currently, we have two broad research targets: 1. Our aim is to synthesize poly(phenylenevinylene) (PPV) analogues involving homo- or hetero-nuclear bonds in the polymer backbone that will conceptually mimic inorganic semiconductors such as gallium phosphide or indium arsenide. 2. We will explore the stability of newly synthesized multiply bonded transition metal-silicon compounds and their potential applications in the fields of catalysis, coordination polymers, conducting materials etc. We will also stabilize metal-free main-group compounds in order to primarily utilize them for small molecule activations and ultimately in catalysis.

Publications

Total number of publications: 18

Selected Publications

- **Majumdar, M.**; Bejan, I.; Huch, V.; White, A. J. P.; Whittell, G. R.; Schäfer, A.; Manners, I.; Scheschkewitz, D. σ–π Conjugated Organosilicon Hybrid Polymers from Copolymerization of a Tetrasiladiene and 1,4-Diethylnylbenzene. *Chem. Eur. J.***2014**, *20,* 9225-9229.
- **Majumdar, M.**; Huch, V.; Bejan, I.; Meltzer, A.; Scheschkewitz, D. Reversible, Complete Cleavage of Si=Si Double Bonds by Isocyanide Insertion. *Angew. Chem. Int. Ed.***2013**, *52,*3516-3520.
- Leszczynska, K.; Abersfelder, K.; **Majumdar, M.**; Neumann, B.; Stammler, H –G.; Rzepa, H. S.; Jutzi, P.; Scheschkewitz, *D.* The Cp*Si^{+} cation as a stoichiometric source of silicon.*Chem. Commun.* **2012**, *48,* 7820-7822.
- Tsurugi, H.; Yamada, K.; **Majumdar, M.**; Sugino, Y.; Hayakawa, A.; Mashima, K. Dinuclear Molybdenum Cluster Catalyzed Radical Addition and Polymerization Reactions by Tuning the Redox Potential of a Quadruply Bonded Mo_2 Core. *Dalton Trans.* **2011**, *40,* 9358-9361.
- **Majumdar, M.**; Sinha, A.; Ghatak, T.; Patra, S. K.; Sadhukhan, N.; Rahaman, S. M. W.; Bera, J. K.Mapping the Transformation $[Ru^{II}(CO)_3Cl_2]_2 \rightarrow [Ru^{II}{}_2(CO)_4]^{2+}$: Implications in Binuclear Water-Gas-Shift Chemistry. *Chem. Eur. J.* **2010**, *16,* 2574-2585.

Awards and Recognitions

- Best Short Lecture Award: 17th International Symposium on Silicon Chemistry (ISOS), Berlin, 2014.
- Krupp-Lehrstuhl fur Allgemeine und Anorganische Chemie: Saarland University, Germany, October 2011 - May 2014.
- CREST Fellowship, Osaka University, Japan, April 2010 - July 2011.
- Toyota Fellowship, Osaka University, Japan, December 2009 - March 2010.

SEEMA VERMA

IISER Fellow

Ph.D.: Indian Institute of Technology, Kanpur, India
Previous position: Adjunct Visiting Faculty- IISER Pune, Project Scientist-NCL, Research Associate-NCL, Lecturer- Pune University
Joining at IISER: July 2009
Email: sa.verma@iiserpune.ac.in
URL: http://www.iiserpune.ac.in/~saverma

Multifunctional Magnetic Nanoparticles

The main research focus of this laboratory is to develop novel synthetic routes to synthesize highly monodispersed multifunctional magnetic nanocrystals using suitable surfactants that are dispersible in both water as well as organic solvents (see Figure 1).

The group has reported a strategy to obtain a stable thin film of magnetic nanocrystals at the air/water interface utilizing Langmuir-Blodgett (LB) method. This strategy can be extended to any similar systems.

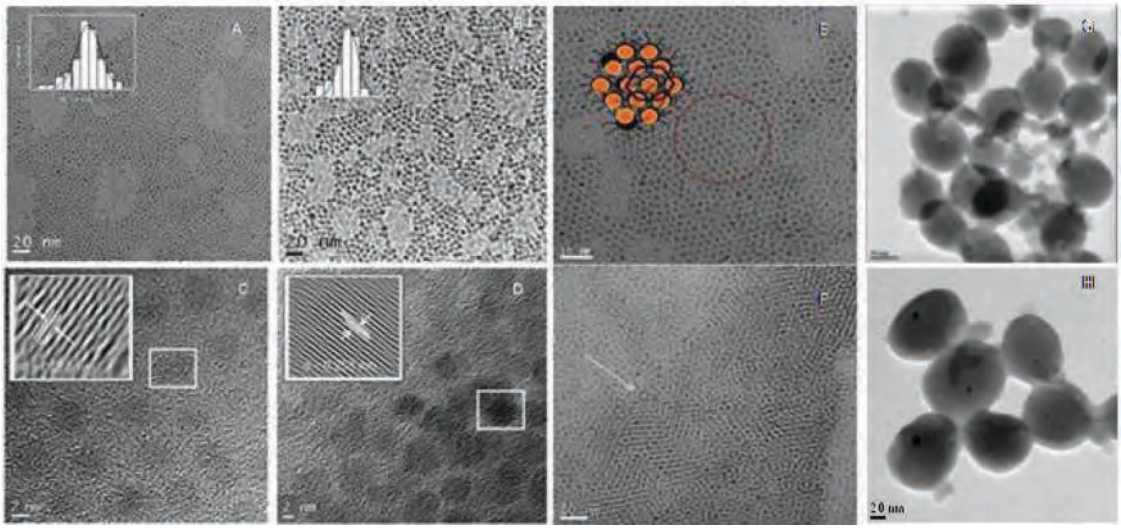


Figure 1: TEM images of (A) $CoFe_2O_4$ and (B) Fe_3O_4 nanocrystals. HRTEM images of (C) $CoFe_2O_4$ and (D)Fe_3O_4 nanocrystals. Inset: Corresponding Lattice fringes of the square marked nanocrystals. (E) and (F): Self assembly for first and second layer of the nanocrystals. (G) and (H) TEM of $CoFe_2O_4$-Ag@mesoporous silica core-shell structure.

The group is also focusing on designing multifunctional magnetic-plasmonic hybrid nanostructures by utilizing novel synthetic routes. Emphasis is given to obtain mesoporous magnetic-plasmonic hybrid materials, suitable for biomedical applications and in active plasmonic devices (see Figure 1 G & H).

A detailed examination of the effect of induced off-stoichiometry on structural, thermal and magnetic properties of nickel cobaltite, nanoparticles has been reported. A comparison of ZFC magnetization of off-stoichiometric ($Ni_{0.75}Co_{2.25}O_4$) and stoichiometric ($NiCo_2O_4$) nanoparticles show stronger exchange interaction value for annealed off-stoichiometric samples.

Publications

Selected Publications

- **Verma, S.;** Kumar, A.; Pravarthana, D.; Deshpande, A.; Ogale, S. B.*; Yusuf, S. M.* Off-Stoichiometric Nickel Cobaltite Nanoparticles: Thermal Stability, Magnetization, and Neutron Diffraction Studies. *J. Phys. Chem. C,* **2014,** *118,* 16246-16254.
- Thampi, A.; Babu K.; **Verma S.** Large Scale Solvothermal Synthesis and a Strategy to Obtain Stable Langmuir–Blodgett Film of $CoFe_2O_4$ Nanoparticles. *Journal of Alloys and Compounds,* **2013,** *564,* 143 –150.
- Kale, S. N.; Jadhav, A. D.; **Verma, S.;** Koppikar, S. J.; Kaul-Ghanekar, R. S.; Dhole, D.; Ogale, S. B. Characterization of Biocompatible $NiCo_2O_4$ Nanoparticles for Applications in Hyperthermia and Drug Delivery. Nanomedicine, Nanotechnology, *Biology and Medicine,* **2012,** *8,* 452-459.
- **Verma, S.;** Joy, P. A.; Kurian, S. Structural, Magnetic and Mossbauer Spectral Studies of Nanocrystalline $Ni_{0.5}Zn_{0.5}Fe_2O_4$ Ferrite Powders: An Effect of Elemental Stoichiometric Coefficients of Combustion Mixture, *J. Alloys Compounds,* **2011,** *509,* 8999-9004.
- **Verma, S.;** Pravarthana, D. One-Pot Synthesis of Highly Monodispersed Ferrite Nanocrystals: Surface Characterization and Magnetic Properties, *Langmuir,* **2011,** *27,* 13189-13197.

External Grants

- Synthesis and self-assembly of magnetic nanostructures: a search for novel phenomena. Funding Agency: DST-SERC under Young Scientist FAST TRACK scheme. (July 2009-August 2011).

Teaching Contributions

Physical Chemistry of Solutions, Solid State Chemistry, Chemistry Lab I- Physical chemistry, Chemistry Lab II- Inorganic Chemistry, Advanced Inorganic Chemistry Laboratory, Laboratory Theory Course

Research Group

Past under-graduate students: D. Pravarthana, Akula VenuMadhav, Arya Thampi, Maddala Bala Gopal

ARVIND ANANT NATU

Visiting Faculty

Ph.D.: Poona University
Post-doc.: Institute of Organic Chemistry Technical University, Berlin, Germany
Post-doc.: Institute of Organic Chemistry Bielefeld University, Bielefeld, Germany
Current position: Visiting Faculty, Chemistry
Joining at IISER: August 2006
Email: aa.natu@iiserpune.ac.in
URL: http://www.iiserpune.ac.in/~aa.natu

Bioorganic Chemistry

Our research interest is to develop novel anti fungal compounds to counter the resistance and the side effects associated with currently available drugs. We have focused not only in the development of new chemical classes of compounds but also to identify novel biological pathways that can be disrupted resulting in the effective control of fungal pathogens. In pursuit of this we have selected Chitin synthase as our initial target because of its presence in all the fungi. A new method for the glycocidation of Nucleoside has been developed and extensively used to introduce the bases into the scaffolds. Many of these compounds have shown encouraging activity using specifically developed Haploinsufficiency assay. Appropriate chemical modifications are in progress.

Other interests

- Outreach programs for the motivation of the students to take up careers in Science Education of; special Children.

Teaching Contributions

Teaching experience at post graduate and graduate level for 20 yrs

Visiting faculty in Dept. of Biotechnology, University of Pune

Visiting faculty in Institute of Bioinformatics and Biotechnology, University of Pune

Visiting faculty in Garware college, Pune

Awards and Recognitions

- DAAD Research Ambassador, India
- Honorary advisor to German academic exchange service
- Fellow of the Maharashtra Academy of Sciences
- Visiting Professor at Bielefeld University, Germany
- Best teacher Award, PVG Pune
- Lead Indian chemistry Olympiad teams to London and Hungary

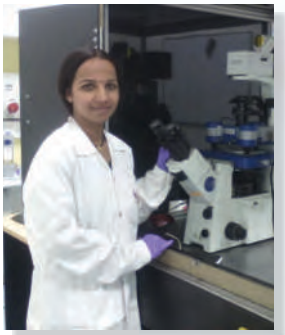
Staff Profile

Mr. Mahesh Jadhav
Designation: Technical Officer
Qualification: M. Sc. (Analytical Chemistry)
Date of Joining: 2 December 2013

Mr. Nitin Dalvi
Designation: Technical Assistant
Qualification: M. Sc. (Organic Chemistry)
Date of Joining: 12 November 2012

Mr. Suresh C Prajapat
Designation: Scientific Assistant
Qualification: M.Sc. (Analytical Chemistry)
Date of Joining: 15 July 2009

Mr. Yathish T. S.
Designation: Laboratory Technician
Qualification: 2nd Pre university course
Date of Joining: 11 March 2013

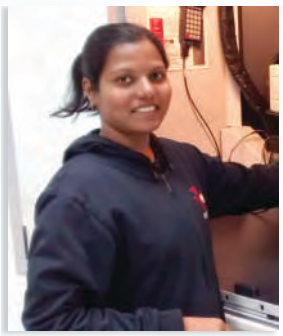


Mrs. Megha K. Paygude
Designation: Laboratory Assistant
Qualification: M.Sc. (Organic Chemistry)
PG diploma in analytical chemistry
Date of Joining: 18 February 2013

Mr. Ganesh Dimber
Designation: Laboratory Assistant
Qualification: B.Com.
Date of Joining: 10 March 2014

Mr. Mayuresh Kulkarni

Designation: Office Assistant
Qualification: B.Com.
Date of Joining: 1 January 2010



Mrs. Archana Shashikant Patil

Designation: Technical Assistant (Single Crystal XRD)
Qualification: M. Sc. (Analytical Chemistry)
Date of Joining: 15 February 2011

Mrs. Swati Manohar Dixit

Designation: Technical Assistant (MALDI)
Qualification: M.Sc. Biotechnology
Date of Joining: 1 July 2011

Mrs. Nayna Ajit Nikam

Designation: Technical Assistant (HRMS)
Qualification: M.Sc. (Analytical Chemistry)
Date of Joining: 20 December 2013

Mrs. Tejasvi Mahendra Tajane

Designation: Teaching Assistant
Qualification: M.Sc. (Analytical Chemistry)
Date of Joining: 24 December 2009

Mr. Mahendra B. Patil

Designation: Teaching Assistant
Qualification: M.Sc. (Inorganic Chemistry)
Date of Joining: 4 January 2010

Ms. Hemlata. S. Phadke

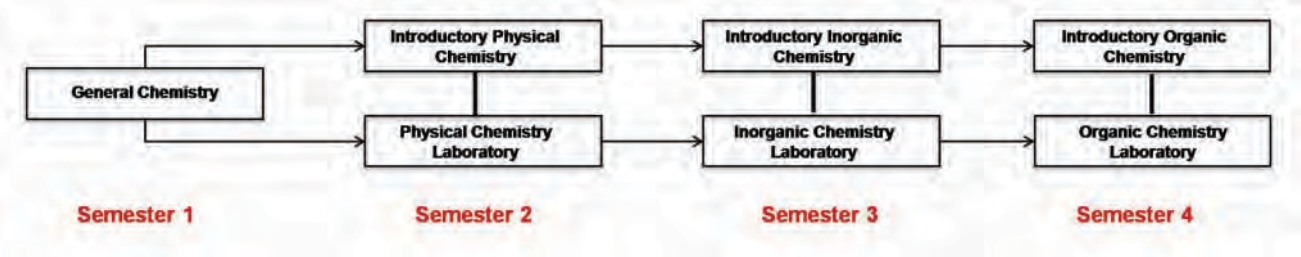
Designation: Teaching Assistant
Qualification: M.Sc. (Organic Chemistry)
Date of Joining: 7 October 2010

UG & Ph.D. Programme

Chemistry Teaching @ IISER Pune

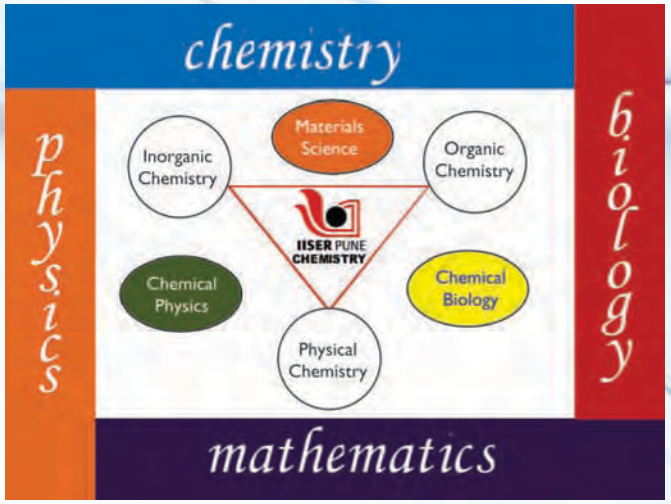
Core courses in the first two years of the BS/MS programme

A first semester course is general chemistry, which would lay the foundations for advanced concepts in chemistry. Here the students would be exposed to a general overview of chemistry in everyday life. Some topics covered include units, measurement, periodicity, thermodynamics, kinetics, bonds, spectroscopy, solutions, chirality and biochemistry. This course serves as the common backbone for the ensuing three semesters of physical, inorganic and organic chemistry, all accompanied by laboratory courses. The laboratory course has been designed to complement the classroom interactions. Together, these seven courses in the first four semesters should sufficiently prepare a student for advanced courses in chemistry and serve as the minimum for anyone who wishes to major in other topics of science such as physics or biology.



The ideology behind the chemistry programme

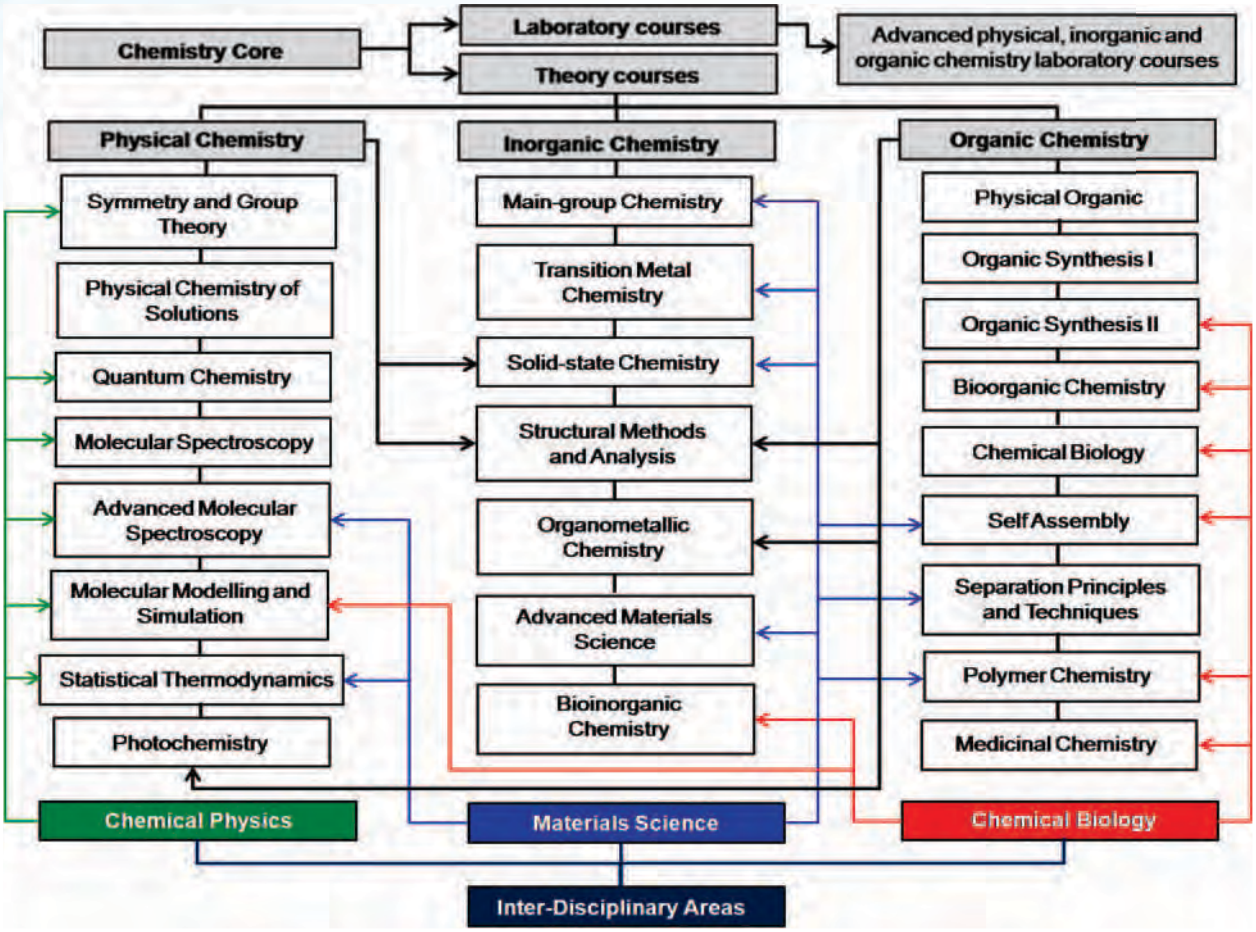
The chemistry programme has been broadly divided into three groups: physical chemistry, inorganic chemistry and organic chemistry. Each semester has at least "core" course (4-credit) from these groups that a student may opt for. They are also arranged in sequence so that all topics in a particular group are covered by the end of the eighth semester. In addition to these core courses, students also have an option of choosing a potpourri of 3-credit courses. These 3-credit courses are not only important for students who wish to major in chemistry but also useful for students who wish to choose chemistry as a minor discipline of interest.



Suggestions to students wanting to "major in Chemistry"

Students who wish to study chemistry as the major subject of interest may opt for a majority of the core courses offered each semester and as many electives as possible in chemistry. Several sequences are available for students to choose from such as organic, inorganic and physical chemistry. If the student is interested in inter-disciplinary areas, one could choose from three available options, materials science, chemical physics and chemical biology. Of course, other combinations of courses yielding the right mix for chemistry and other disciplines might also be possible. In addition, students are allowed to register for two lab/theory projects during their third and fourth years as an elective course.

A flow chart describing all the available courses under each branch of chemistry and their relationship(s) to the inter-disciplinary areas of research is given below.



Interdisciplinarity in Chemistry

Inter-disciplinary courses are divided roughly into three streams:

1. Chemical Physics: These cover courses in the interface of physics and chemistry and include Symmetry and Group Theory, Advanced Molecular Spectroscopy, Statistical Thermodynamics, Quantum Chemistry and Solid State Chemistry. When combined with suitable physics courses, a student might have a good exposure to both chemistry and physics.

2. Chemical Biology: Several courses in the interface of chemistry and biology are offered by the chemistry division. Starting from the sixth semester, a sequence of courses of Bioorganic Chemistry, Chemical Biology and Medicinal Chemistry can complement relevant course in biology division to cover advanced topics in the interface of these two streams.

3. Materials Science: Courses offered under this broad section would cover areas that are common to chemistry, physics and to some extent biology. Starting from fifth semester a series of courses such as Self-assembly in Chemistry, Solid-state chemistry, Polymer chemistry and Advanced materials chemistry will give good insights to relevant courses both in physics and biology. Further, the courses offered under this section would be useful to all the students who want to specialize in any branch of organic, inorganic or physical chemistry.

Credit System:

4 credits: Typically, there will be three lectures a week. Often instructors devote 2 lectures for theory and 1 lecture for tutorial. In addition, assignments, self-study and group exercises would be part of the course.

3 credits: Typically, there will be two lectures a week. In the senior years, these courses require solid background in the prerequisites mentioned for the course. Advanced laboratory courses are 3 credits with 3 lab hours per week.

2 Credits: Laboratory courses in the first four semesters are two credits each with 3 hours per week.

CHM 101: General Chemistry (3 Credits)

Introduction: This course would be introductory to other major courses in Inorganic, Organic and Physical Chemistry. It would cover the fundamental concepts from the physical, inorganic and organic chemistry branches of chemistry and would be taught in a way to provide link between the 12th grade Science and the undergraduate General Chemistry.

Topics: Chemistry in the Modern World, Measure of Matter, The Mole, Error Analysis, Introduction to Thermodynamics, Chemical Equilibrium, Chemical Kinetics, Behaviour of Gases, Properties of Solutions, Solubility, Understanding Acid-Base Buffers, Solid State- Crystal vs Amorphous Solids, Symmetry and Organisation Principles for Crystalline Solids, Unit Cell, Periodicity of Elements, Periodic trends in properties of the Elements, Types of Bonds, Lewis Dot Structures, Introduction to Organic Chemistry, Chirality, Functional groups and structural diversity, conformational analysis, Hetero atoms and Metals in Chemistry and Biology Applications, Reactive intermediates, Organic Materials, Asymmetric Synthesis, Chemistry of Life- Peptides, Nucleic acids, Carbohydrates, Lipids.

References:

1. *Chemistry: Principles, patterns and applications*, by Bruce A. Averill and Patricia Eldredge, Publisher: Prentice Hall, Ed. 2007.
2. *An introduction to error analysis: The Study of Uncertainties in Physical Measurements*, John Robert Taylor, 2nd Ed.
3. *Chemical Principles*, by Steven S. Zumdahl (6^{th} Ed. Year 2009)
4. *The Biological Chemistry of the Elements*, F. D. Silva and Williams, Oxford University Press

Prerequisites: None

CHM 102: Physical Chemistry (3 Credits)

Introduction: This course will deal with the basic principles of physical chemistry like thermodynamics, chemical kinetics, kinetic theory of gases and quantum mechanics. The physical chemistry concepts taught in this course will also serve as an important tool to understand reactions and mechanisms in organic, inorganic and biochemistry and principles of spectroscopy. At the end of this course, students should be able to apply these physical chemistry concepts to study various phenomena in physics, chemistry, materials science and biology.

Topics: Chemical kinetics: Basic laws of kinetics, Experimental determination of reaction order and rate, Study of

fast reactions, Simultaneous reactions, Temperature dependence of reaction rate, Mechanism of chemical reactions; **Kinetic Theory of Gases:** Maxwell's distribution of molecular velocities, collision in a gas, mean free-path, heat capacity of gases, Equi-partition of energy, viscosity, thermal conductivity, Impact on environmental science and astrophysics; **Thermodynamics:** State and path functions, Internal Energy, Heat and Work, Laws of thermodynamics, Heat Capacity, Enthalpy, Entropy, Gibbs Free energy, Gibbs Helmholtz Equation, Chemical Potential, Colligative properties; **Chemical Bonding & Spectroscopy:** Historical development, Schrödinger equation and Postulates of Quantum Mechanics, Operators in Quantum Mechanics, Particle in a 1 D Box to 3 Dimensional Box, Harmonic Oscillator, Hydrogen atom, Molecular Orbital Theory and Valence Bond Theory, Applications in Spectroscopy.

References:

1. Physical Chemistry by Gordon M. Barrow
2. Physical Chemistry by I. N. Levine
3. Physical Chemistry by P. W. Atkins
4. Quantum Chemistry by Donald A. McQuarrie
5. Quantum Chemistry by I. N. Levine
6. Chemical kinetics by Keith J. Laidler

Prerequisites: None

CHM 121: Physical Chemistry Lab-I (2 Credits)

Introduction: This course is designed to acquaint the students with the practice of experimental physical chemistry. The goal of the labs is to provide modest introductions to the core area of scientific activity which would help the students to apply the principles of thermodynamics, kinetics and spectroscopy presented in the physical chemistry lecture course, in some illustrative experiments. Students are encouraged to understand the interconnection between the experimental foundation and the underlying theoretical principles and appreciate the limitations inherent in both theoretical treatments and experimental measurements. Students will gain familiarity with a variety of measurement techniques which will help them to understand the methods to develop the laboratory skills and the ability to work independently, instil good attitudes and habits towards knowing the safe way of doing science.

Topics: Acid Base Titration using pH meter, Acid Base Titration using conductivity method, Potentiometric titrations, Heat of Neutralization, Kinetic Study of Ester hydrolysis, Activation Parameter calculations, Colligative properties of Solutions, Optical Activity by Polarimetry, UV - VIS Spectrophotometry

References:

1. Experiments in Physical Chemistry, Carl W. Garland, Joseph W. Nibler, David P. Shoemaker, Eighth edition
2. *Physical Chemistry*, Peter Atkins, Julio de Paula, Eighth edition

Prerequisites: None

CHM 201: Introductory Chemistry II: Inorganic Chemistry (3 Credits)

Introduction: This course will introduce the students the most rudimentary principles behind the chemistry of inorganic compounds. In this course an overview introduction to the common elements of the periodic table from alkali metals to noble gases through transition-metal and main group elements will be given and their property such as periodicity, structure and bonding, acidity and basicity, redox reactivity etc. will be discussed. At the end of the course, the students should be able to derive the structure of various covalent compounds, apply the concept of acid-base chemistry to various reactions and as a whole understand the importance of the elements of the periodic table for living matter.

Topics: Atomic Structure, electronic configuration, periodicity, sizes of atoms and ions, ionization energy, electron affinity, relativistic effects, chemical bonding, Lewis theory, valance bond and molecular orbital theories, solid state

structures and properties, concepts of acids and bases, Brønsted and Lewis theory, hard and soft acids and bases, oxidation and reduction, electrode potentials, Nernst equation, representation of electrochemical data, importance of water splitting, batteries and fuel cells, coordination complexes, theories of bonding in transition metal compounds, some introduction to main group compounds.

References:

1. *Inorganic Chemistry*, Shriver and Atkins, Oxford University Press, International Student Edition, 4th Edn., 2006
2. *Concepts and Models of Inorganic Chemistry*, B. Douglous, D. McDaniel and J. Alexander, Wiley- India Edition, 3rd Edn., (student edition), 2006
3. *Inorganic Chemistry* by Huheey, Keiter, Keiter and Medhi, Pearson Education, 4th Edn. 2007

Prerequisites: None

CHM 221: Introductory Chemistry II: Inorganic Chemistry (3 Credits)

Introduction: This laboratory course aims at demonstrating experimentally the concepts that are introduced in the introductory inorganic chemistry course that will run parallel to this lab course. Experiments based on some of the key topics that are introduced in the theory courses such as acids and bases, redox chemistry, chemistry of coordination and main group compounds will be carried out enhancing a further understanding to these topics. Through these experiments the students not only will have a complete knowledge of these topics but also will learn the use of various techniques such as analytical and spectroscopic methods to study them.

Topics: Acid-base titrations relevant to the neutralizing power of antacids, conventional and photochemical synthesis of coordination compounds, complexametric and spectroscopic estimation of metal ion concentrations in coordination compounds, redox titration relevant to the iodine content in common salts, synthesis of disinfectants containing main group compounds such as Alum, soaps and micelles.

References:

1. ***A Collection of Interesting General Chemistry Experiments, by*** A. J. Elias, revised ed., Universities Press (India) Pvt. Ltd., 2007.

Prerequisites: None

CHM 202: Introductory Organic Chemistry

Introduction: This course includes structural chemistry of organic compounds with an emphasis on electronic structure, reactivity, conformation and stereochemistry. These concepts will prepare students for a mechanistic-based approach to learning organic reactivity. Emphasis will be given towards developing problem-solving skills unique to organic chemistry.

Topics: Carbon compounds and chemical bonding, Reactive Intermediates; Carbocations and Carbanions chemistry, Free radicals and Carbenes, Acidity, basicity, and pKa, Acidity, The definition of pKa, Basicity, Factors that influence the acidity and basicity, HSAB Principle, Stereochemistry: R and S descriptors, Axis of Chirality; E and Z system; erythro, threo; Helical descriptors- M and P. cis, trans, Conformational analysis of ethane and cyclohexane, Addition Reactions: Nucleophilic addition reaction: Nucleophilic addition reation to carbonyl group: Molecular orbitals explain the reactivity of the carbonyl Group, angle of nucleophilic attack on aldehydes and ketones, Electrophilic addition reactions: Alkenes react with bromine, water; bromohydrin formation etc. Conjugate addition: Conjugation changes the reactivity of carbonyl group, Alkenes conjugated with carbonyl groups, Substitution Reactions: Nucleophilic substitution at saturated carbon: Nucleophilic substitution**,** Structure and stability of carbocations, The SN1 and SN2 mechanisms for nucleophilic substitution. Neighbouring group participation (NGP), Aromatic electrophilic and nucleophilic substitutions, Elimination Reactions: Types of elimination reactions and factors that affecting the elimination reactions. Rearrangements: Various types: Electrophilic and nucleophilic rearrangement and Migratory aptitudes, Free radical rearrangements and Pericyclic rearrangements.

References

1. *Organic Chemistry* Clayden, J.; Greeves, N.; Warren, S.; Wothers, P. Oxford University Press, 1st Edition. (Primary)
2. *Organic Chemistry* by Solomons, John Wiley & Sons Inc; 2nd or 3 rd edition
3. *March's Advanced Organic Chemistry* by M. Smith and J. March, Wiley-Interscience; 5, or 6 edition

CHM 222: Organic Chemistry Lab (2 credits)

Introduction: This laboratory course will provide opportunity for the students to learn the nuances in organic synthesis. Students will be trained to setup reactions, monitor reactions by functional group analysis and by thin layer chromatography. In this course, students will learn basic separation and purification techniques (e.g., filtration, recrystallization and column chromatography) that are commonly used in organic synthesis. Students will be also trained in isolating natural products from natural sources. Furthermore, students will characterize the synthesized or isolated compounds by determining the melting point or by IR, UV and NMR spectroscopy. Together this organic chemistry lab course will set a platform for students who wish to pursue research in experimental chemistry.

Topics: Functional group analysis, classical name reactions and oxidation, reduction, cycloaddition, aromatic electrophilic substitution reactions, isolation of natural products and synthesis of fluorescent compounds, purification techniques such as recrystallization and column chromatography.

Prerequisite: None

CHM 311: Physical Organic Chemistry (4 Credits)

Introduction: The main objective of this course is to expose students to the fundamental concepts of structure and function in organic reactions. The use of kinetics and thermodynamics to elucidate mechanisms of reactions will be dealt with. At the end of this course, students will be in a position to predict reactivity patterns and propose reasonable mechanisms.

Topics: Basic concepts of acidity, basicity, and pKa; Equilibria, kinetics and mechanisms; Rearrangements; Radical Reactions; Mechanisms in Biological Chemistry; Advanced Molecular Orbital Theory; Sterochemistry and conformational analysis; Thermal pericyclic reactions; Sigmatropic and electrocyclic reactions; Synthesis and Reactions of carbenes.

References:

1. *Organic Chemistry*. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P. Oxford University Press, 1st Edition. (Primary)
2. *Modern Physical Organic Chemistry*, Anslyn, E.; Dougherty, D. A.; 1st edition, **2006**. University Science Books
3. *Advanced Organic Chemistry, Part A: Structure and Mechanism*, Sundberg, R. J.; Carey, F. A. 4th Edition. Kluwer/Plenum Press, **2000**
4. *Physical Organic Chemistry*, Isaacs, N. 2nd Edition, Addison-Wesley-Longman, 1995

Prerequisites: None, but this course is prerequisite for Organic Synthesis I and II.

CHM 312: Main group chemistry (4 Credits)

Introduction: The objective of this course is to focus on the chemistry of main group elements such as hydrogen, alkali metals and P-block elements from group 13 – 18 of the periodic table. The central theme of this course is to give a detailed account on the fundamental concepts relevant to structure and bonding, acids and bases, redox behavior, reactions and applications of the main group elements and their compounds. In addition to providing a necessary foundation for inorganic chemistry, this course will also emphasize the role of main group compounds in multi disciplinary areas of chemistry such as supramolecular, organometallic, materials science and catalysis.

Topics: Theories of bonding, acids and bases, thermodynamic acidity parameters; hydrogen and classical hydrogen bond, water, hydrates, hydrogen ions, metal hydrides, activation of hydrogen complexes; alkali metals in liquid

ammonia; boron, boranes, carboranes, borazines and borates; allotropy of carbon; silane and polysilanes, silicone Polymers, silicates; compounds of nitrogen, activation of nitrogen, nitrogen fixation, hydrogen, halogen, oxygen and nitrogen compounds of phosphorous; oxygen and singlet oxygen, ozone, complexes of molecular oxygen; N-S compounds; sulphides, oxides and oxoacids of sulphur, chalcogenides and polychalcogenides; halogens, polyhalides, interhalogen compounds, charge-transfer complexes of Halogens; Compounds of Xenon and other noble gases; Zintl compounds and homometallic clusters; elemental and compound semiconductors; energy, polarity, and reactivity of M-C bond; organometallic chemistry of the main group elements.

References:

1. *Advanced Inorganic Chemistry* by Cotton, Wilkinson, Murillo and Bochmann (6th Ed.).
2. *Chemistry of the Elements* by Greenwood and Earnshaw (2nd ed.)
3. *Inorganic Chemistry*, Shriver and Atkins, Oxford University Press, International Student Edition, 4th Edn., 2006
4. *Inorganic Chemistry* by Huheey, Keiter, keiter and Medhi, Pearson Education, 4th Edn. 2007.

Prerequisites: None

CHM 320: Symmetry and Group Theory (4 credits)

Introduction: The objective of this course is to recognize symmetry in molecules and understand its role in chemistry. The course will explore the role of symmetry in (A) determining molecular properties like optical activity and dipole moment (B) classifying and assigning nomenclature to molecules, molecular states and molecular motions, (C) bringing about simplifications in the application of quantum mechanics to molecules and (D) determining spectroscopic selection rules based on molecular symmetry. Group theory applied to the study of molecular symmetry has far reaching consequences in chemistry and the course will provide an in-depth appreciation of this.

Topics: Symmetry elements and operations, *Schönflies notation* of point group, prediction of dipole moment and optical activity from the viewpoint of symmetry, definition of group, subgroup and class, matrix representation of a point group, reducible and irreducible representations, great orthogonality theorem and its corollaries, construction of character tables and meaning of all the terms in a character table, Mulliken symbols for irreducible representations, direct product of irreducible representations, application of symmetry to quantum mechanics, application of symmetry to spectroscopy – electronic, IR and Raman selection rules, projection operator and its application to symmetry adapted linear combinations, construction of molecular orbital correlation diagram of simple and complex molecules, Hückel π molecular orbital of a conjugated system.

References:

1. Chemical Applications of Group theory: F. A. Cotton (Wiley Interscience)
2. Molecular symmetry and group theory: R. L. Carter (John Wiley & Sons)
3. Symmetry and Spectroscopy: D. C. Harris and M. D. Bertolucci (Dover)
4. Group Theory and Quantum Mechanics: Michael Tinkham (Dover)

Prerequisites: None. Strongly recommended for students planning to take Quantum Chemistry and Molecular Spectroscopy

CHM-331: Self-assembly in Chemistry (3 Credits)

Introduction: This chemistry course is aimed to provide fundamental aspects of self-assembly in chemistry and its application for supramolecular architectures. This course is beneficial for students who are interested in molecular materials, nanomaterials, biology-chemistry interface and self-assembly in chemical and biological systems. The course also consists of student's seminars on selected topics, problem solving, and idea generation and laboratory experiments on making and testing of self-assembled objects.

Topics: Introduction to self-assembly and supramolecular chemistry, types of non-covalent interactions, importance

of pre-organization, determination of association, problem solving, metal ion-macro-ligand supramolecular structures and metallo-supramolecular polymers. Single & self-complementary system, two, three and four and multiple arm hydrogen bonding systems, switching of recognition functions, hydrogen bonded supramolecular polymers, etc. Guest-host approaches in cyclodextrins, Calixarenes, Molecular rings & Nots, Rotaxanes and Dendrimers with examples. Anionic, cationic and neutral Micelles, critical micelle concentration (CMC) determination, bolaamphiphilies and application of micelles in drug delivery, etc. Origin of liquid crystals, mesogens self-organization, Types: nematic, smectic and cholestric liquid crystals and characterization of LC-materials. Self-assembly in DNA, protein and peptides.

References

1. Selected Topic covered in Comprehensive Supramolecular chemistry, Volume-8
2. Core concepts in Supramolecular chemistry and Nano-chemistry: Authors; J. W. Steed
3. Supramolecular chemistry: Fundamentals and applications: Advanced Text book: Authors: Katsuhiko Ariga
4. Introduction to Soft mater: Synthetic and Biological Self-Assembling Materials: Authors: Ian W. Hamley
5. Review and research articles, communications and notes published in international journals (will be provided).

CHM332: Separation principles and Techniques (3 Credits)

Introduction: Separation plays a crucial role in Chemistry and Biology, where sample purity is of utmost importance e.g. Pharmaceuticals, Biopharmaceuticals and Fragrances etc. In this course, we will learn theory and practice of separation. We will have hands on training on HPLC, GC, GC MS, Centrifugation, Electrophoresis and few other Chromatographic techniques.

Topics: Thermodynamics, diffusion rates, mass transfer etc. Solvent extraction, distillations, liquid-liquid extraction and other methods of separation. Types of Chromatography: GC, HPLC, hyphenated techniques. Electrophoresis, centrifugation DNA/Protein separations / purifications. Green Separation process separation using zeolite and polymer membranes. Chiral separations, molecular recognition, molecule imprinting and polymer separations.

References:

1. An Introduction to Separation Science: B.L. Karger; L.R. Snyder and C. Horvath.
2. Handbook of Separation Process Technology: R.W. Rousseau.
3. Separation Process Principles: J.D. Seader and E.J. Henley.

Prerequisites: None

CHM340: Advanced Organic Chemistry Lab

Introduction: This laboratory course will provide reasonable opportunity for the students to learn the nuances in organic synthesis. Classical name reactions, rearrangements and multi-step reactions will be performed in this course. Purification techniques such as column chromatography will be also included. Synthesized compounds will be characterized using IR, UV, NMR and Mass spectrometer. Put together this organic chemistry lab course will set a platform for students who wish to pursue research in experimental chemistry.

Topics: Separation of ternary quantitative analysis of organic compounds. Electrophilic aromatic substitution reactions: Synthesis of methyl orange (organic dye); Name reactions and rearrangements: Wittig reaction, Beckmann rearrangement: Acetanilide from Acetophenone Oxime; Multi step synthesis: Synthesis of substituted Flavones and characterization of the diketo intermediates and flavones derivatives; Photochemical reaction: Photochemical reaction: Synthesis of benzopinacol from benzophenone using sunlight; Thermal pericyclic reactions: Diels alder reaction: anthracene and maleic anhydride; Cupper(I) mediated cycloaddition reaction: Click reaction: Azide and alkyne coupling reaction; Organometallic reactions: Palladium catalyzed cross-coupling reaction: Stereochemistry: Addition of Bromine to trans-cinnamic acid.

References

1. Experimental procedures will be provided from current literature.
2. ***A Collection of Interesting General Chemistry Experiments*** by Anil J. Elias, Revised Edition 2007, Universities Press.
3. *Comprehensive Practical Organic Chemistry* by V. K. Ahluwalia, Renu Aggarwal, 2000, Universities Press.
4. *Vogel's Textbook of Practical Organic Chemistry (5th Edition)*, Publisher: Prentice Hall

CHM 310: Quantum Chemistry (4 credits)

Introduction: The objective of this course is to understand the fundamental principles of quantum mechanics as applied to molecular model systems and molecules. Students taking the course will get an understanding of the theoretical principles underlying molecular structure, bonding and properties. The concepts discussed in this course will be useful to the students who wish to pursue research in areas of theoretical and computational chemistry, spectrsocpy, molecular biology and materials science. The course will start with a discussion of the Schrödinger equation and exact solutions to various one-body problems followed by approximate methods to solve the many-body electronic problem.

Topics: Introduction to quantum mechanics, wave equation and Schrodinger equation, postulates of quantum mechanics, particle in a box, harmonic oscillator, rigid rotor, hydrogen atom, variational principle, perturbation theory, introduction to many electron systems, electron spin, antisymmetry, Slater determinants, 2-e system, Valence Bond theory, Molecular Orbital theory, Huckel theory, Hartree-Fock theory, post Hartree-Fock methods.

References:

1. *Quantum Chemistry* by Donald A. McQuarrie
2. *Modern Quantum Chemistry* Attila Szabo and Neil Ostlund
3. *Quantum Chemistry* by Ira N. Levine

Prerequisites: None

CHM 321: Organic Synthesis-I (4 Credits)

Introduction: This course primarily deals with various strategies involved in logical organic synthesis by incorporating basic organic transformations, reactions, and reactivity. Various functional group transformations, reagents, and reaction mechanisms, will be discussed to provide students a clear understanding and importance of organic synthesis. This course should serve as a stepping stone for students looking to progress to more advanced synthetic concepts and methodologies.

Topics: The concept of protecting functional groups, oxidations and reductions in functional group transformations, enantioselective reduction and oxidation, diastereofacial selectivity in acyclic systems, The chemistry of carbon-carbon sigma and pi bonds and related reactions: Reactions of Carbon-Carbon Double and triple bonds, formation of carbon-carbon single, double and triple bonds and rings, chemistry of enolates, Organometallic Reagents in organic syntheses.

References:

1. *Advanced Organic chemistry* Part B: Francis A. Carey and Richard J. Sundberg, Springer
2. *March's Advanced Organic Chemistry* M. Smith and J. March, Wiley-Interscience
3. *Organic chemistry* J. Clayden, N. Greeves, S. Warren, P. Wothers, Oxford University Press
4. *Modern Organic Synthesis An Introduction* Zweifel and Nantz, W. H. Freeman and Company

Prerequisite: CHM 311: Physical Organic Chemistry

CHM 322: Transition Metal Chemistry (4 Credits)

Introduction: The objective of this course is to provide a detailed account to the chemistry of transition metals and emphasize their relationship to other multi-disciplinary topics such as bioinorganic chemistry and organometallic

chemistry. The central theme of this course is to focus on the fundamental concepts needed to understand the transition metal chemistry relevant to their structure, bonding, properties such as spectral characteristics, reactivity, stereochemistry etc. This course will be useful to all those students who have opted for chemistry as a major subject. At the end of this course, students will also learn about the role of transition metals in several other fields like materials science, biology and catalysis.

Topics: Crystal and ligand field theories, crystal field stabilization energies, Irving-Williams series, 10Dq and pairing energies, molecular orbital diagrams for coordination complexes, magnetic susceptibilities and Jahn-Teller effects. Spectroscopic terms, LS-coupling scheme, ligand field transitions, charge transfer bands, selection rules, Orgel diagrams, Tanabe-Sugano diagrams and circular dichroism. Thermodynamic and kinetic factors, labile and inert complexes, ligand substitutions in octahedral and square planar complexes, stereo chemical effects. Oxidation/reduction potentials, Nernst equation and redox stability in water, complementary and non-complementary redox reactions, Inner and outer sphere electron transfer and Marcus theory, electron transfer in metalloprotiens. Basic terminologies, kinetic factors affecting quantum yield, photochemistry of Co, Rh, Cr and Ru.

References:

1. *Inorganic Chemistry*, Shriver and Atkins, Oxford University Press, International Student Edition, 4th Edn., 2006
2. *Inorganic Chemistry* by Huheey, Keiter, keiter and Medhi, Pearson Education, 4th Edn. 2007
3. *Reaction Mechanisms of Inorganic & Organometallic Systems*, R. B. Jordan (3rd Edn.), Oxford University Press, 2007

Prerequisites: NIL

CHM 323: Fundamentals of Spectroscopy (4 Credits)

Introduction: The objective of this course is to teach the fundamentals of major branches of Spectroscopy and its applications. Spectroscopy is an important research tool in all areas of science (Chemistry, Physics and Biology) to determine the structures of molecules. In principle, the interaction of light with matter provides a great deal of physical information about a system of interest and ultimately defines many of the observational techniques used. In this course, this radiation-matter interaction and the quantitative information it can provide about molecular systems will be examined.

Topics: Introduction to radiation-matter interaction, Rotational Spectroscopy, Infrared Spectroscopy, Raman Spectroscopy, Electronic Spectroscopy, Nuclear Magnetic Resonance (NMR) Spectroscopy, Electron Spin Resonance (ESR) Spectroscopy.

References:

1. Introduction to Molecular Spectroscopy: G. M. Barrow, McGraw-Hill
2. Fundamentals of Molecular spectroscopy: C. N. Banwell and E. M. McCash, 4th edition, Tata McGraw Hill
3. Modern spectroscopy, J. M. Hollas (Wiley, New York)
4. Spectra of atoms and molecules, P. F. Bernath (Oxford University Press, New York)
5. Physical Chemistry - A Molecular Approach; Donald A. McQuarrie and John D. Simon, Viva Books Private Limited
6. Physical Chemistry, P. W. Atkins, Oxford University Press

Prerequisite: NIL

CHM 334: Physical Chemistry of Solutions (3 Credits)

Introduction: This course is designed to teach elementary physical chemistry of solutions to have an insight on the thermodynamic treatment of the chemical problems. Special emphasis will be given to the study of stability in macroscopic systems undergoing phase change and rigorous calculations of equilibrium properties of solutions will be undertaken. Numerical problems related to equilibrium properties, colligative properties, transport properties, conductivity, mobility, viscosity etc. will be taken care to have hands on experiences. Apart from the familiarity with the routine thermodynamic calculations of chemical systems, students would be exposed to contemporary areas such as

ionic liquids, polymer and gel electrolytes, chemical sensors, biosensors, Fuel cells with emerging application potential.

Topics: Thermodynamic Description of mixtures, Partial Molar Quantities, Ideal Solutions, Nonideal solutions, Gibbs-Duhem Relation, Equilibrium constant for solutes, vapour-pressure lowering, Application to biology and polymer science, Electrolytes in Solution, Ionic Liquids, Ionic Mobilities, Dielectric Effect, Ionic Strength, Dissociation of Weak Electrolytes, Debye-Huckel Theory, Activities in more Concentrated Solutions, Polymer and Gel electrolyte, Thermodynamic description of Electrochemical Cells, Nernst equation, Activity Coefficients from EMF's, Equilibrium Constant from EMF's, Chemical Sensors, Fuel Cells, Impact on Biochemistry, Phase Equilibria, Pressure-Temperature Phase Diagrams, Phase Rule, Immiscible Liquids, Eutectic Formation, Solid-Compound Formation, Three-Component, Solid-Liquid Systems, Liquid-vapor, Pressure-Composition Diagrams, Boiling-Point Diagrams, Distillation, Adsorption of Gases, Supercritical fluids, Impact on Materials Science.

References:

1. Physical Chemistry by P. W. Atkins and Julia de Paula, eighth edition
2. Physical Chemistry by Gordon M. Barrow, fifth edition
3. Physical Chemistry by I. N. Levine, fifth edition
4. Modern Electrochemistry by Bockris and Reddy, second edition

Pre requisites: Essentials of Physical Chemistry covered during 1st and 2nd semester

CHM351: Bioorganic Chemistry (3 Credits)

Introduction: This course is intended to provide a basic knowledge on the biosynthesis of biomolecule precursors and natural products. The content of this course is a chemistry-based approach to understanding the basic structure, reactivity, biological functions and biosynthesis of precursors–amino acids, nucleotides, fatty acids, lipids and secondary metabolites. This course is also a preamble for Chemical biology course offered in the 8th semester.

Topics: Overview of basic structure of carbohydrates, nucleic acids, proteins, and lipids, Primary and secondary metabolism, bioenergetics, biological and organic reaction mechanisms, coenzymes and cofactors, amino acids: biosynthesis of amino acids promoted by pyridoxal phosphate, Shikimic acid pathway to aromatic amino acids, peptides, depsipeptides antibiotics and their biological activities, biosynthesis of nucleosides.beta-oxidation of fatty acids, biosynthesis of fatty acids, various lipids, polyketides, prostanoids, leucotrienes and other secondary metabolites, metabolites of mixed biosynthetic origin, from acetate, mevalonate and shikimate pathway, isoprenoids: isoprene unit, monoterpenes, diterpenes, sesquiterpenes and triterpenes, and biological activities, steroids: steroidogenesis, biosynthesis and biological implications.

References:

1. *Principles of Biochemistry,* Lehninger, 4th edition
2. *Biochemistry*, Voet and Voet, 3rd edition

Prerequisite: None

CHM 360: Advanced Inorganic Chemistry Lab (3 Credits)

Introduction: This course aims at the integration of chemical synthesis and spectral characterization techniques. Reactions studied in lectures would be explored in laboratory conditions to rationalize synthesis and structural aspects of inorganic molecules and coordination complexes. In this process, students will be encouraged to use advanced instrumentation such as IR and UV-Vis spectrophotometers apart from advanced technique such as multi-nuclear NMR spectroscopy.

Topics: Spectrochemical studies for analysis and stoichiometry, redox reactions. Synthesis, characterization, spectral and magnetic properties of metal co-ordination complexes having different oxidation numbers; determination of their spin-only magnetic moments, Determination of halide concentration by non-spectroscopic methods. Synthesis and

evaluation of properties for a silicon polymer, Optical properties of coordination complex. Single crystal-growth and X-ray crystal structural determination.

References:

1. Experimental procedures will be provided from current literature.
2. *A Collection of Interesting General Chemistry Experiments, by A. J. Elias revised ed., Universities Press (India) Pvt. Ltd., 2007*
3. *Vogel's Qualitative Inorganic Analysis*, 7th Edition, Revised by G. Svehla, Publisher: Prentice Hall

Prerequisite: None

CHM 410 Advanced Molecular Spectroscopy (4 Credits)

Introduction: The modern avatar of spectroscopy is a highly interdisciplinary one. Applications are in subjects as diverse as Chemistry, Physics, Astronomy, Material science and Biology. The developments in spectroscopy now span from ultrafast time-scales to micro and millisecond regimes and a wide range of spatial length scales. The objective of this course is to teach spectroscopy at the advanced level and familiarize the students with the capabilities of these advanced tools. The students will learn fundamentals of laser operation, different types of laser systems, optical techniques that use lasers and various advanced spectroscopic techniques. The students will get practical training in analysis of spectral data. Modern research topics relevant to this course will be provided to the students and they will make a presentation on that topic at the end of the semester. This course will be useful for those who would like to use advanced spectroscopic techniques in their research.

Topics: Introduction to interaction of radiation with matter, Fundamentals of lasers and laser systems, Advanced spectroscopic techniques and applications, e.g., Raman spectroscopy, Electronic spectroscopy, Fluorescence techniques, Cavity ringdown absorption spectroscopy, Supersonic jet spectroscopy**,** Laser induced fluorescence, Stimulated emission pumping, Multiphoton ionization spectroscopy, Photoelectron spectroscopy, Ultrafast spectroscopy.

References:

1. Modern spectroscopy, J. M. Hollas (Wiley, New York)
2. High Resolution Spectroscopy, J. M. Hollas,(Butterworth, London)
3. Laser fundamentals: W. T. Silfvast (Cambridge University press, Cambridge)
4. Laser Chemistry: Spectroscopy, Dynamics and Applications by H. H. Telle, A. G. Urena, R. J. Donovan (Wiley)
5. Physical Chemistry - A Molecular Approach; Donald A. McQuarrie and John D. Simon, Viva Books Private Limited
6. Spectra of atoms and molecules, P. F. Bernath (Oxford University Press, New York)

Prerequisites: CHM 323: Fundamentals of Spectroscopy

CHM 411: Organic Synthesis-II (4 Credits)

Introduction: Builds enough knowledge for independent planning of the total synthesis of an organic molecule. This course would develop research skills and critical thinking by application of course content to practical problem solving. In addition, the course introduces student to variety of strategies in which a molecule can be conceived depending on the intuition of the student. Total synthesis of several molecules from the literature will be discussed in detail which gives students firm understanding of the facts for planning their own synthesis endeavours.

Topics: Formation of carbon-carbon single bonds, Organometallic reagents, synthesis of carbocyclic systems, sketches of synthesis, tactics in organic synthon approach, disconnection approach for multiple step syntheses, functional group interconversions, synthesis of heterocycles: ring-closing reactions; asymmetric synthesis, chiral pool synthesis, chiral auxillary, organocatalysis, Desymmetrisation, total synthesis of natural products.

References:

1. *Organic chemistry* by Jonathen Clayden, N. Greeves, S. Warren, P. Wothers Oxford University Press, 1st edition
2. *Organic Synthesis, the Disconnection Approach,* Warren, S. G. New York : Wiley, 2nd edition

3. *The Logic of Chemical Synthesis* by E. J. Corey & Xue-Min Cheng
4. *Classics in Total Synthesis* by K C Nicolaou & Sorensen
5. *Advanced Organic Chemistry, Parts A and B,* Francis A. Carey and Richard J. Sundberg, Springer, 5th Ed.
6. Other course material given time to time from literature.

Prerequisites: Organic Synthesis-I (CHM321)

CHM 413: Bioinorganic Chemistry (4 Credits)

Introduction: This course will explore the inorganic chemistry behind the requirement of biological cells for metals such as zinc, iron, copper, manganese, and molybdenum. The course comprises of principles of coordination chemistry and spectroscopy topics such as EPR and Mossbauer for metal ions. The reactivity of coordination complexes of metal ions will be discussed in the context of the reaction mechanisms of specific metalloenzymes. A portion of the course will be devoted to the toxicity of metals and also their utility in drugs and in diagnostic agents.

Topics: General aspects of chemistry of dioxygen, Fe, Cu and Co. Nature of M-O2 linkage, heme proteins, molecular mechanism of oxygenases, catalase and peroxidase, Cu-Zn superoxide dismutase. Electron transferases, Respiration, Photosynthesis, Nitrogen fixation and Vitamin B12. Fe-S proteins, redox behaviour. Metals for diagnosis and chemotherapy, Pt anti-cancer drugs as a case study. ESR and Mossbauer spectroscopy.

References:

1. *Bioinorganic Chemistry*, Bertini, Gray, Lippard and Valentine, Viva Books
2. *Biological Inorganic Chemistry*, Bertini, Gray, Stiefel, Valentine, University Science Books
3. *The Biological Chemistry of the Element*,: F. D. Silva and Williams, Oxford University Press

Prerequisites: CHM 322: Transition Metal chemistry

CHM430: Advanced Physical Chemistry Laboratory (3 credits)

Introduction: This course offers a mix of experimental and computational experiments based on the physical concepts in chemistry. Experiments offered in this course provide students an opportunity to learn advanced instrumentation techniques as well as its application to study a variety of chemical problems. The computational experiments are based on the theoretical principles taught in quantum chemistry and symmetry and group theory. The computational experiments are designed to show how computations can be used to predict, complement and validate experimental results.

Topics: Building of molecules using Gaussview: Calculation of energy, structure and vibrational frequencies using Gaussian software,Visualization of geometry, orbitals, vibrations and spectra using Gaussian software, Contact angle measurement on hydrophobic and hydrophilic surface, Synthesis and spectroscopic characterization of metallic nanostructures, Raman spectroscopic studies of CCl_4, Lithographic patterning, Study of an oscillatory reaction by Emf, or (and) absorbance measurement, To study the fluorescence quenching of Anthracene by CCl_4 in n-hexane or (and) ethanol.

References:

1. *Experimental Physical Chemistry* by V. D. Athawale, Parul Mathur; New Age International Publisher.
2. Relevant research papers in J. Chem. Educ.
3. Gaussian 03/09 User manual

Prerequisites: None

CHM 431: Chemical Biology (3 Credits)

Introduction: Chemical biology is a discipline that integrates principles and experimental techniques drawn from both chemistry and biology to understand biological phenomena. This course will use topics from the current literature to

provide an overview of Chemical Biology and will demonstrate the integration of chemical, biochemical and biological approaches. Also, this course will cover the use of modern instrumentation for studying various aspects of biological systems, including structure, dynamics and functions. The course structure will empower both chemists and biologists by providing chemists with relevant new biological targets and biologists with useful new chemical tools.

Topics: Chemical and enzymatic modification of nucleic acids, solid-phase peptide synthesis, unnatural amino acids and their incorporation. Biomolecular interactions: protein-nucleic acid, protein-small molecule, nucleic acid-small molecule and sugar-protein. Combinatorial approaches to drug discovery, high-throughput screening, chemical glycomics and various biophysical techniques.

References:

This course will use topics from the current literature, and appropriate reference information will be provided to the students.

1. Nucleic Acids in Chemistry and Biology, Edt. Michael Blackburn, Michael Gait, David Loakes and David Willaims, 3rd Edition, 2006, RSC Publishing
2. Chemical Biology, a practical course: Herbert Waldmann, Petra Janning. 1st Edition, 2004, Wiley-VCH
3. Chemical Biology: From small molecules to systems biology and drug design. Edt. Stuart L. Schreiber, Tarun Kapoor, Gunter Wess. Volume 2, 2007, Wiley-VCH

Prerequisite: None

CHM 432: Solid State Chemistry (3 Credits)

Introduction: This course is designed to provide the fundamental knowledge of the crystallography, structure and properties. The objective of this course is to lay the foundation for understanding the relationship between the internal structure of matter and the properties of materials that make them attractive for applications. Apart from the familiarity with the routine structure – property correlations, students would be exposed to some of the most recent developments across the spectrum of Solid – State and materials, while at the same time reflecting on key turning points in the evolution of this scientific interdisciplinary course and projecting the knowledge into the directions for future research progress.

Topics: Crystal Structure, Fundamentals of lattice, unit cell, atomic coordinate, Bravais Lattices, Crystal's direction and planes, Symmetry operations, symmetry elements, Point Group, Space group, Crystal Structures, Representation of Crystal Structures, Crystal Diffraction, lattice Vibrations, Electronic Properties and Band theory of solids, metals, insulators and semiconductors, Electronic structure of solids-bond theory, k space and Brillouin zones, Magnetic Properties, Magnetic moment, Curie law, Curie-Weiss law, Mechanism of magnetic ordering, Exchange Interaction, Domain theory, Hysteresis, Anisotropy, Ferromagnetism, Ferrimagnetism, Antiferromagnetism, Classical and Quantum mechanical treatment, Dielectric and Optical Properties, Polarization, Depolarization field, Local electric filed at an atom, Ferroelectric domains, Piezoelectricity, Ferroelectricity, Selected examples of materials, structures, properties and applications with respect to structure/property relations, Recent developments, Thermal Analysis, Thermogravimetric analysis (TGA), differential thermal analysis (DTA) and differential scanning calorimetry, Materials processing and Performances.

References:

1. Basic Solid State Chemistry by A. R. West, second edition, John Wiley & Sons, Ltd.
2. Solid State Chemistry and its applications by A. R. West, John Wiley & Sons, Ltd.
3. Solid State Physics by N. W. Ashcroft and N. D. Mermin; CBS Publishing Asia Ltd.
4. Introduction to Solid State Physics by Charles Kittel; John Wiley and Sons
5. New Directions in Solid State Chemistry, by C.N.R.Rao and J. Gopalakrishnan,1997, Cambridge University Press
6. Atomic and electronic structure of solids by E. Kaxiras, Cambridge University Press (2003)

Pre requisites: Essentials of Physical and Inorganic Chemistry covered during 1st and 2nd semester.

CHM 436: Molecular Modeling and Simulation (3 Credits)

Introduction: This course will introduce theoretical concepts and computer based experiments on Molecular Dynamics simulations and quantum mechanical methods. A strong background in mathematics and physics is recommended for students of this course. Students with research interest in theoretical and computational chemistry/physics are expected to benefit from this course.

Topics: Introduction to Molecular Dynamics: Atomic potentials and force-fields, periodic boundary conditions, equation of motion integrators, treatment of statistical mechanical ensembles, time correlation functions, radial distribution functions, mean square displacement, diffusion coefficient. Perform simulation experiments using GROMACS Molecular Dynamics software. Learning Molecular Builder and Visualization Tools (Gaussview, MOLDEN and Visual Molecular Dynamics). Quantum Mechanics: Born Oppenheimer Approximation, Self Consistent Field Theory/Density Functional Theory Equations, Basis Sets, Electron Correlation, Use of Quantum Chemistry software (GAUSSIAN).

References:

1. Computer Simulations of Liquids, M. P. Allen and D. J. Tildesley, Oxford Science Publications, 1987
2. Molecular Modelling: Principles and Applications, Andrew R. Leach, Addison Wesley Publishing Company, 1997
3. Introduction to Computational Chemistry, Frank Jensen, John Wiley & Sons, 2007
4. Density Functional Theory of Atoms and Molecules, R. G. Parr and W. Yang, Oxford University Press

Pre-requisites: None

CHM 420: Structural Methods and Analysis (4 Credits)

Introduction: The objective of the course is to develop the foundation for important characterization methods (spectroscopic and analytical methods) used routinely by organic/inorganic/physical chemists. Understanding of principles followed by problem solving sessions involving discussions of spectral data of known and unknown compounds is expected to develop critical thinking and problem solving skills. The course is also important for biology students who want to pursue their research in the chemical biology.

Topics: Infrared Spectroscopy, Ultra-Violet Spectroscopy, Fluorescence Spectroscopy, Elemental Analysis, Mass Spectrometry, Nuclear Magnetic Resonance and multiple problem solving sessions for structure elucidation of natural and synthetic molecules.

References:

1. *Spectrometric Identification of Organic Compounds* by R. M. Silverstein, F. X. Webster & D. J. Kiemle. 7th Edition
2. *Organic Spectroscopy*, William Kemp, 3rd Edition. W.H. Freeman & Company
3. *Introduction to Organic Spectroscopy*, L. M. Harwood & T. D. W. Claridge, 1st Edition (Oxford Chemistry Primers nº 43), Oxford University Press, Oxford, 2000)
4. *Principles of Fluorescence Spectroscopy* by J. R. Lakowicz, 2nd Edition, 2004, Springer
5. *Introduction to Mass Spectrometry,* Watson, J. T.; Sparkman, O. D. Wiley, 4th edition
6. *Mass Spectrometry a Textbook*, Gross, J. H. Springer

Prerequisites: None

CHM 421: Polymer Chemistry (4 Credits)

Introduction: This course's emphasis is to provide fundamental knowledge in polymer science. This course is very important for all the students who wish to learn and practice macromolecular and organic chemistry. New physical chemistry concepts in macromolecules, organic synthetic methodologies for polymers and applications of polymers in the industrial applications will be focused. This course is beneficial for students who are interested in polymeric materials, nanomaterials, biology-chemistry interface and macromolecular assemblies in chemical and biological systems.

Topics: Basic concepts, Molecular weight distribution, Linear, Branched, Cross-linked, grafted- Polymers, Polymer Crystallization, Glass Transition, Solution and Melt viscosity, Polymer Rheology, Step-polymerization, Addition Polymers, Radical, Cationic, Anionic Living polymerization, Block copolymers, Liquid crystalline polymers, Ring opening polymerization, Physical and Reactive blends, Nano-composites and synthetic-natural fiber composites, Concepts of conducting polymers and their applications in opto-electronics and sensors, one and 3D dimensional polymeric materials. Dendrimers, hyperbranched polymers, random branched polymers, branching density, influence of branching on the melt, viscosity, rheological and thermal properties of polymers.

References

1. *Principles of Polymerization*, 4th Edition, G. Odian, Wiley
2. *Text Book of Polymer Science*, Billmeyer Jr., Wiley
3. *Polymers: Chemistry and Physics of Modern Materials*, J. M. G. Cowie, Wiley
4. Review and research articles, communications and notes published in international journals (will be provided)

Prerequisites: None

CHM 422: Statistical Thermodynamics (4 Credits)

Introduction: Statistical thermodynamics provides a measure to understand classical thermodynamics (energy, entropy, free energy etc.) from microscopic motion of atoms (position, velocity). Therefore, this course provides the tools to explain certain phenomena that are governed by classical thermodynamics (e.g., free energy) from a molecular point of view. The basis of molecular dynamics simulation, which covers a complete research area, is based on statistical thermodynamics. The course requires basic knowledge of mathematics and the concept of probability. This course is essential for a physical chemistry student. However, the knowledge in general will help other branches as well, especially those who would like to think in terms of atoms and molecules. This course will be eventually helpful to pursue a theoretical/computational research.

Topics: Thermodynamics postulates, Conditions of equilibrium, Reversible Processes and Maximum Work Postulate, Extremum Principle, Maxwell Relation, Review of Probability Theory, Ensembles and Postulates, Canonical Ensemble, Grand Canonical Ensemble, Microcanonical Ensemble, Other Ensembles, Equivalence of Ensembles, Thermodynamic Connection, Fluctuation, Boltzmann Statistics, Fermi-Dirac Statistics, Bose-Einstein Statistics, monatomic gas, monatomic crystals, Ideal Diatomic Gas, Classical Statistical Mechanics, Ideal Polyatomic Gas, Chemical Equilibrium, Distribution Functions in Classical Monoatomic Liquids.

Reference:

1. H. B. Callen, Thermodynamics and Introduction to Thermostatistics, 2nd Edn, (1985). First six chapters
2. Statistical Mechanics, Donald A McQuarrie, University Science Books, California, USA, Viva Books Private Limited, New Delhi (Indian Edn) [First 7 chapters and some other chapters)
3. An Introduction to Statistical Thermodynamics, Terrell L. Hill, Dover Publications, Inc, New York

Prerequisite: Basic mathematics

CHM 433: Photochemistry (3 Credits)

Introduction: This course will give idea to students how light can take a major role in many natural and chemical processes. Here the students will also get thorough knowledge about excited state processes (e.g. fluorescence, phosphorescence etc.) and the importance of the above mentioned processes in all fields of science.

Topics: The laws of photochemistry, Primary processes in photochemical reactions, Fluorescence and phosphorescence, Concept of quantum yield, lifetime, anisotropy, Techniques used in measuring fluorescence lifetime, Quenching phenomenon, Electron Transfer Reaction & Marcus Theory, Fluorescence resonance energy transfer (FRET), Concept of Excimer and exciplex, Diffusion controlled rate constants, Flash photolysis, Some typical photochemical reactions: Olefin isomerization, Retinal and Rhodopsin photochemistry of vision, Acid-base

chemistry, Reversal of pericyclic selection rules, Woodward-Hoffman rules of electrocylic reactions, photocycloaddition reactions, UV-DNA damage, breaking aromaticity, Di-Π methane rearrangement, oxadi-Π-methane rearrangement, Photochemistry of carbonyl compounds, Norrish type I and Norrish type II reactions, Nitrobenzyl photochemistry, Paterno-Buchi reaction, azo compound and diazocompounds, diazirins, azides and photoaffinity labeling, Chemiluminenscence and Chemiluminescent reactions, light sticks, photodynamic therapy, photochemistry of transition metal complexes and photosynthesis.

References:

1. Modern Molecular Photochemistry by *Nicholas J. Turro*
2. Principles of Fluorescence Spectroscopy by *J. R. Lakowicz*
3. Handbook of Photochemistry by Marco Montalti, Alberto Credi,, M. Teresa Gandolfi
4. Physical Organic Chemistry by Eric V. Anslyn, D. A. Dougherty
5. Synthetic Organic Photochemistry by A. G. Griesbeck

Prerequisite: Fundamentals of Spectroscopy (CHM202)/Molecular Spectroscopy

CHM 434: Medicinal Chemistry (4 Credits)

Introduction: This course is intended to provide insights into applications of organic chemistry in the field of drug discovery and development. In this course, approaches to new drug discovery including natural product isolation, high-throughput synthesis and screening, and rational drug design will be discussed. We will also compare and contrast these methods of drug discovery and development. We will also learn approaches to lead identification followed by structure-activity determination for optimization of a drug's activity. Some modern methods of drug delivery including formulations and prodrug approaches will be briefly discussed. Finally, we will present a brief introduction to pharmacology, target identification, pre-clinical and clinical development of a drug candidate.

Topics: Enzyme structure and catalysis, types of inhibitors, inhibitors as the basis for drug design, receptors, drug-receptor interactions, ion channels, natural products with drug-like activity, DNA damaging and intercalating agents, RNA-based methods, drug metabolism, biodistribution, drug delivery methods, prodrugs.

References:

1. *An Introduction to Medicinal chemistry*, Graham Patrick, Oxford University Press, USA; 3 rd or 4th edition
2. *The Organic Chemistry of Drug Design and Drug Action*, Richard Silverman Academic Press; 2nd edition
3. Principles of Biochemistry, Lehninger, 4th edition

Prerequisite: None

CHM 441: Advanced Materials Science (3 Credits)

Introduction: This course would be in two parts. Whist the first part would give an overview of Materials and discuss the structure-property relationships in materials from fundamental perspectives. The second part would introduce you to practical methods and techniques of investigating the properties of these materials for energy applications. Throughout the course there would be sufficient references to state-of-the-art materials and prototypes.

Topics: Overview of Novel Materials, Types of Solids- Metals, Alloys, Insulators, Polymers, Semiconductors, Composites, Liquid Crystals, Quasi Crystals, Defects in Solids – Point, Line and Volume or Bulk Defects, Phase Transformations and Phase Equilibria, Solid Solution, Non-Equilibrium Cooling, Eutectic Systems Properties of Materials- Mechanical, Thermal, Optical and Magnetic. Adsorption Fundamentals, Concepts and Application, Adsorption Kinetics, Chemistry and Physics of Conduction, Primary and Secondary Batteries, Types of Batteries-Charging vs Discharging, Chargeable vs Non-Rechargeable Sources. Physical Limitations of Battery Performance. Solar Cells – Principle, Working and Tuning. Impedance Spectroscopy- Methods for Conductivity Meaurements, Electrochemical Kinetics- Butler Volmer Equation, Fick's First Law Of Diffusion, Tafel Equation. Fuel Cells- Design and Measurement, Types of Fuel Cells, Structure of Porous Electrolytes, Electrode Kinetics. Carbon Materials-

Nanotubes, Fullerenes, Graphenes as Advanced Functional Materials.

References:

1. *Adsorption by Powders and Porous Solids: Principles, Methodology and Applications* (J. Rouquerol et al.)
2. *Modern Batteries, Second Edition*, C. Vincent, Bruno Scrosati
3. *An Introduction to Physics of Solar Cells: From Basic Principles to Advanced Concepts*, by Peter Würfel, John Wiley & Sons, 2009
4. *Fuel Cell Fundamentals*, by Ryan O'Hayre, Suk-Won Cha, Whitney Colella, Fritz B. Prinz
5. *Electrochemical Methods: Fundamentals and Applications*, by Allen J. Bard, Larry R. Faulkner

Prerequisites: CHM-320: Symmetry and Group Theory and CHM-432: Solid State Chemistry

CHM 442: Organometallic Chemistry: Principles and Applications (3 Credits)

Introduction: The main goal of this course is to help the students to learn the principles of organometallic chemistry with emphasis to the understanding of their structure, properties and applications. Organometallic chemistry has served as a bridge between traditional inorganic and organic chemistry and contributed to the development of several important discoveries in synthetic organic chemistry. At the end of this course students will have a thorough understanding of the classification and mechanistic aspects of several organometallic reactions and will be able be identify the role of organometallic complexes in organic synthesis and industrial applications. This course will be also useful to Ph.D students working in the area of organic and inorganic chemistry.

Topics: Concepts of structure and bonding: definition, 18 electron rule, classes of ligands, bonding and structural considerations. Fundamental reaction process: oxidative addition and reductive elimination; insertion and elimination; ligand substitution processes, transmetallation, nucleophilic and electrophilic addition and abstraction. Preparative and characterization methods: general methods for the preparation of organometallic compounds and spectroscopic and analytical techniques for the elucidation of structure, properties and reactivates. Synthetic applications: coupling reactions, cyclization reactions, addition reactions, carbonylation, Pauson-Khand reaction, olefin oxidation, carbenes and activation reactions. Industrial applications: hydrogenation, hydroformylation, isomerization, metathesis and polymerization reactions. Bio-organometallics: nitrogen fixation, coenzyme B12, hydrogenase, CO dehydrogenase and methanogenesis.

References:

1. Ch. Elschenbroich, A. Salzer, Organometallics; 2nd Ed. VCH, 1995
2. Robert H. Crabtree, Organometallic chemistry of the transition metals, 4th Edition, Wiley-Interscience

Prerequisite: None

CHM 301/302/401/402: Lab/Theory Project (3 Credits)

Introduction: The larger objective of this course is to encourage students to participate in ongoing research at IISER. This may be in the form of a reading/literature review/theoretical or computational project/lab based research project.

Topics: The student has to identify, talk to and mutually agree on a research project before registering for this course. The scope, duration, structure, expectations, and evaluation criteria (also see below) for the course are decided by the project supervisor.

References: As per suggestions of the project supervisor.

1. The course is open to Int. B.S./M.S. students in the 5-8th semesters.
2. CGPA $\geqslant$ 6.5 till the previous semester.
3. Project can be carried out only in IISER.
4. Requires prior permission of the faculty concerned.

Prerequisite: NIL

BS-MS, Integrated PhD (I-PhD) & PhD Students Chemistry Course Details*

Course code	Name of the Course	Students	2008	2009		2010		2011		2012		2013		2014	
			Fall	Spring	Fall	Spring	Fall	Spring	Fall	Spring	Fall	Spring	Fall	Spring	Fall
CHM 310	Quantum Chemistry	BS-MS	9				31		22		60		19		22
		Int. Ph.D.								6		9		5	
		Ph.D.				4				5		5		9	
CHM 311	Physical Organic Chemistry	BS-MS	17		11		16		35		13		23		24
		Int. Ph.D.							6		8		5		10
		Ph.D.	5		4		3		3				1		2
CHM 312	Main Group Chemistry	BS-MS	10		11		15		33		16		22		
		Int. Ph.D.							6		8		5		35
		Ph.D.							3						
CHM 330	Advanced Organic Chemistry Lab	BS-MS			8		8		26		13		23		17
		Int. Ph.D.							6		8		8		10
		Ph.D.													
CHM 331	Self-assembly in Chemistry	BS-MS	10		18		16		43		32		35		46
		Int. Ph.D.							6		11		5		
		Ph.D.			6		7		14		8				
CHM 332	Separation Principles & Techniques	BS-MS	15		12		11		14		17		25		37
		Int. Ph.D.							6		8		7		11
		Ph.D.									12		7		11
CHM 320	Symmetry and Group Theory	BS-MS		14		21			48		18		19		26
		Int. Ph.D.							6		8		5		10
		Ph.D.		2		5					9		2		4
CHM 321	Organic Synthesis I	BS-MS		14		8		13		27		18		18	
		Int. Ph.D.								6		8		5	
		Ph.D.		2		4		3		1		3		3	
CHM 322	Transition Metal Chemistry	BS-MS		12		14		20		41		41		33	
		Int. Ph.D.								6		8		5	
		Ph.D.						3		6		4		5	

*Number of students opting the course in each semester

Course Code	Name of the Course	Students	2008	2009		2010		2011		2012		2013		2014	
			Fall	Spring	Fall	Spring	Fall	Spring	Fall	Spring	Fall	Spring	Fall	Spring	Fall
CHM 333	Electro Chemistry	BS-MS		8											
		Int. Ph.D.													
		Ph.D.													
CHM 350	Advanced Physical Chem Practical-II	BS-MS		13											
		Int. Ph.D.													
		Ph.D.													
CHM 351	Bioorganic Chemistry	BS-MS		4		12		15		25		26		29	
		Int. Ph.D.								4		2		2	
		Ph.D.		3		4		8		8		5		4	
CHM 333 CHM 334	Physical Chem. of Solution	BS-MS						16		33		20		17	
		Int. Ph.D.								5		6		3	
		Ph.D.												2	
CHM 360	Advanced Inorganic Chem. Lab	BS-MS				12				25		18		17	
		Int. Ph.D.								6		8		5	
		Ph.D.													
CHM 330	Advanced Organic Chem Lab	BS-MS			8		8		26		13		23		17
		Int. Ph.D.							6		8		8		10
		Ph.D.													
CHM 410	Adv. Molecular Spectroscopy	BS-MS			9		9		10		35		18		19
		Int. Ph.D.									6		9		5
		Ph.D.			2		1		6		7		2		8
CHM 411	Organic Synthesis II	BS-MS			9		9		10		23		13		14
		Int. Ph.D.									6		9		5
		Ph.D.			9		8		2				4		13
CHM 412	Adv. Inorganic Chemistry	BS-MS			10		9		11						
		Int. Ph.D.							2						
		Ph.D.													
CHM 430	Advanced Physical Chem. Lab	BS-MS	12*		12		7		7		33		17		4
		Int. Ph.D.									6		9		5
		Ph.D.													

Course Code	Name of the Course	Students	2008	2009		2010		2011		2012		2013		2014	
			Fall	Spring	Fall	Spring	Fall	Spring	Fall	Spring	Fall	Spring	Fall	Spring	Fall
CHM 431	Chemical Biology	BS-MS			4		2		9		21		10		19
		Int. Ph.D.									6		5		
		Ph.D.			10		6		10		10		8		15
CHM 432	Solid State Chemistry	BS-MS			11		9		14		23		16		21
		Int. Ph.D.									4		8		4
		Ph.D.					6		6		7		4		4
CHM 420	Structral Methods & Analysis	BS-MS				11		4		10		30		20	
		Int. Ph.D.										3		6	
		Ph.D.												8	
CHM 421	Polymer Chemistry	BS-MS				10		11		14		50		19	
		Int. Ph.D.										1		2	
		Ph.D.				6		1		2		4		3	
CHM 422	Statistical Thermody -namics	BS-MS				10		6		4		11		15	
		Int. Ph.D.										7		2	
		Ph.D.													
CHM 423	Medicinal Chemistry	BS-MS				6		9		10		24		13	
		Int. Ph.D.										1		5	
		Ph.D.				4		7		6		5			
CHM 433	Photochemistry	BS-MS				13		9		10		37		19	
		Int. Ph.D.										7		3	
		Ph.D.				5		1				2		5	
CHM 435	Bio-inorganic Chemistry	BS-MS				5		8							
		Int. Ph.D.													
		Ph.D.													
CHM 436	Molecular Modeling & Simulation	BS-MS				2		5		5		11			9
		Int. Ph.D.								1		3			1
		Ph.D.								12		2			2
CHM 442	Organometallic Chemistry	BS-MS										19		17	
		Int. Ph.D.										4		6	
		Ph.D.										5		6	
CHM 413	Bio-inorganic Chemistry	BS-MS									34		16		26
		Int. Ph.D.									6		8		
		Ph.D.									2		1		2

BS-MS Chemistry Thesis*

Sl. No.	Name of the Student	Thesis Title	Thesis Supervisor
MS Thesis-2011			
1	Haritha Rao	Synthesis and enzymatic incorporation of an azide -modified uridine triphosphate analogue	Dr. S. Srivatsan
2	Kumar Saurav	Synthesis of gamma-ammino beta-keto esters and the study of biomolecular interactions using ITC	Dr. H. N. Gopi
3	Harpreet Singh	Banana and star shaped liquid crystalline oligo-(phenylenevinylene)s	Dr. M. Jayakannan
4	Prakhar Arora	Synthesis & charaterization of macrocycles based on thiophenes subunits chemistry	Dr. V. G. Anand
5	Vedant Pande	Investigation of non-covalent interactions in mixed clusters of heterocyclic aromatic compounds: A supersonic jet study combined with quantum chemistry calculations	Dr. Aloke Das
6	D. Pravarthana	Multifunctional magnetic nanoparticles for biomedical applications	Dr. Seema Verma
7	Shishir Suresh Chourey	Design and synthesis of JNK1 allosteric inhibitors	Lupin Industry
8	Rakesh Gaur	Synthesis of thiophene based macrocycle and metal dipyrrins	Dr. V. G. Anand
9	Ashutosh Priyadarshi	Design towards the synthesis and evaluation of naphthalenediimide based anion sensors	Dr. Pinaki Talukdar
10	Hutashan Vajpeyi	Study of water dynamics in the DNA-daunomycin intercalation pathway	Dr. Arnab Mukherjee
11	Varun Kumar Rishi	Ab initio quantum chemical study of selenium dioxide mediated allylic hydroxylation of alkenes	Dr. Sudip Roy (NCL)
MS Thesis-2012			
1	Sandeep Gupta	Bitumen: Chemical composition and rheological behaviour	Shell, Bangalore
2	Dharmraj Robins Chourasia	Analysis of product patents in pharmaceuticals for mailbox applications granted by Indian patent office during 2005-06 to 2009-10	Dr. Raj Hirwani (URDIP, Pune)
3	Rohit Kumar	A density functional theory study of structure, stability and reactivity of Clathrate hydrates	Dr. Arun Venkatnathan
4	Neha Agrawal	Synthesis and characterization of hybrid peptides containing gamma- and vinylogous amino acids	Dr. H. N. Gopi

*Project done during the 5th year of BS-MS Programme

Sl. No.	Name of the Student	Thesis Title	Thesis Supervisor
5	Anuj Bisht	Development of conducting polyaniline-gold nanocomposites	Dr. M. Jayakannan
6	Amitosh Sharma	Design, synthesis, characterisation and host-guest interaction studies of p-stacking self assembled porous organic framework	Dr. Sujit K. Ghosh
7	Prashant Agrawal	Bitumen- organo-clay composites	Shell, Bangalore
8	Abhinaw Kumar	Interaction of polyethylenimine with phospholipid bilayer at different pH: A molecular dynamics study	Dr. Sudip Roy (NCL Pune)
MS Thesis-2013			
1	Piyush Agarwal	Pair-wise dispersive corrections of an optimally-tuned range-separated hybrid functional	Prof. Leeor Kronik (Wiezmann Institute, Israel)
2	Sumeet Kumar Singh	Probing the stability of designed coiled-coil motifs using small synthetic fluorescent amino acids	Dr. H. N. Gopi
3	Nishant Singh	Design and synthesis of J and H aggregates of glycyrrhetinic acid esters as low molecular weight organogelators	Dr. Vijay Gadgil HUL, Bangalore
4	Shreyas Supekar	Sequence dependent localized distribution of various water dynamics in the grooves of DNA	Dr. Arnab Mukherjee
5	Anup Ingole	Study of interaction between fluorescent dyes and cucurbituril host in aqueous solution	Dr. Partha Hazra
6	Amit Kumar	Synthesis, properties and photochemistry of organomodified polymers	Dr. Ashish Vaidya Hindustan Unilever, Bangalore
7	Iti Kapoor	A diversity oriented synthesis pathway for leodoglucomide analogues	Dr. Srinivas Hotha
8	Rohan Kumbhare	Design, synthesis and evaluation of scaffolds for thiol-mediated tunable drug release	Dr. Harinath Chakrapani
9	Uma Sridhar	Dextrin vesicles and their encapsulation capabilities for drug delivery	Dr. M. Jayakannan
10	Suhas Shahaji Gawali	Synthesis and characterization of inhibitor loaded nanoparticles for temporal targeting of PI3K signalling	Dr. S. Basu
MS Thesis-2014			
1	Shweta Singh	Structure-Property correlation studies of – donor based MOF	Dr. Sujit K. Ghosh
2	Koturkar Deepali Madhusudan	Synthesis and characterization of polymeric nanoparticles for dual drug delivery in cancer.	Dr. Sudipta Basu
3	Vikas Negi	DFT based study of methanation in the presence of subsurface atomic hydrogen on Co (0001) surface	Dr. Aarthi Thyagarajan, Shell Technology, Bangalore

Sl. No.	Name of the Student	Thesis Title	Thesis Supervisor
4	Vikash Kumar	Development of π - conjugated polymer sensors and organic phosphors for luminescent materials	Dr. M Jayakannan
5	Rupesh Kumar Xaxa	Spreading behavior of oil-in-water emulsion on model solid substrates	Dr. Sudipta Ghosh Dastidar
6	Sreejith Varma J	Synthesis of acryl amidines via intramolecular amino group migration	Dr. Pinaki Talukdar
7	Upendra Singh	Synthesis of nanomaterials and their composites for energy conversion and storage	Dr. Satishchandra Ogale, NCL Pune
8	Anurag Agrawal	Synthesis, incorporation and fluorescence of base modified Peptide Nucleic Acid (PNA) manomers	Dr. S. G. Srivatsan
9	Indra Kumar Mahawar	Synthesis of thiophosphoramide and phosphoramide ligands and reactivity studies with metal ions	Dr. Boomi Shankar
10	Sumit Bhatnagar	Cost effective synthesis of metaloxides/sulphides for enhanced supercapacitor application	Dr. Satishchandra Ogale, NCL Pune
11	Vivek Kumar	Biophysical Aspects of Binding Interaction between Anticancer Drugs and G-Quadruplex	Dr. Partha Hazra
12	Ravi Raja Adhikari Panda	Nucleophilic addition on glycosyl 1,2-orthoesters of pyranose and furanosoyl sugars	Dr. Srinivas Hotha
13	Amrit Kumar	Design, synthesis, characterization and host-guest interaction studies of triazine based covalent organic frameworks	Dr. Sujit Ghosh
14	P. Sudheer Kumar	Theoretical study of structural changes in DNA under high external hydrostatic pressure	Dr. Anirban Hazra
15	Digvijay Porwal	Multicomponent reactions involving arynes, phosphine and N-substituted Isatins	Dr. A Y Biju, NCL Pune
16	Shada Arun Dixith Reddy	Chloro bridged Palladium (II) hexamers supported by tris imido phosphate tri-anions and studies of their catalytic evaluations	Dr. R Bhoomi Shankar
17	Aditi Jakhar	Novel multi-coded molecular recognition motifs for fully extended programmed molecular self-assembly	Dr. G J Sanjayan, NCL Pune
18	Akula Venumadhav	Design strategy to magnetic-plasmonic nanohybrids	Dr. Seema Varma
19	Raya Rahul Kumar	Design and Synthesis of New porphyrin based COF containing intramolecular H-bonding for the enhancement of stability and crystallinity	Dr. Rahul Banarjee, NCL Pune
20	Vimlesh Kumar Bind	Supramolecular phthalocyanine aggregates	Dr. Nirmalya Ballav
21	Rajkumar Yadav	Synthesis & characterization of [14]Thiatriphyrin (2.1.1) and crystallization & physical properties of thiatripyrrine co-crystals	Dr. V. G. Anand
22	Bhaisare Rupal Dinesh	Mild and biocompatible synthesis of highly symmetric tetra-substituted pyrazine from amino acid and peptides: A novel strategy for self-stapling of peptide	Dr. H. N. Gopi

Sl. No.	Name of the Student	Thesis Title	Thesis Supervisor
23	Vemulapalli Louwkhyaa	Synthesis and characterization of insulin mimetic vanadyl complexes and their binding studies with BSA	Prof. Devadas Manwal, Osmania University
24	Ankita Malik	Synthesis and utilisation of β -hydroxy α-amino acids (Statines) in the design of hybrid peptide foldamers and their biological applications	Dr. H. N. Gopi
25	Sher Singh Meena	Nucleation and growth of ZnO on different surfaces and study of their functional properties	Dr. Amitava Pramanik, Uniliver R&D, Banglore
26	Vivek Verma	Synthetic and botanical mosquito repellent and their antibacterial activity in PAN membrane	Dr. K Balasubramanian, Defence Institute of Advance Technology, Pune
27	Kush Kumar Upadhyay	Synthesis of metal oxides/sulfides and porous carbon for energy storage application	Dr. Satishchandra Ogale, NCL Pune
28	Siddharth Chopra	Composite materials for shoe soles	V. B. Parvatikar, Footwear Design and Dev. Inst., Noida
29	Pilli Veena	Enhanced dispersion of catalytic phases on metal oxides	Dr. M. Madhusudhan Rao, Shell Technology Centre, Banglore
30	Abhishek Singh	Interaction and Fabrication of OPV functionalized SWNT optical sensors	Dr. Harsh Chaturvedi
31	Abhishek Meena	Fe-TAML encapsulated MSN as biomimic peroxidas for picomole detection of proteins	Dr. Sayam Sengupta, NCL Pune
32	Pramod Kumar	Synthesis and evaluation of charged PNA analogues/ conjugates for improved DNA/RNA binding selectivity and better cell entry	Prof. K. N. Ganesh
MS Thesis-2015			
1	Mahitha M. K.	Application of nanoscale materials in analytical mass spectrometry	Prof. T. Pradeep, IIT Madras
2	Aswathi Ashok	Plasmonics and magnetic properties in doped semiconductor nanocrystals	Dr. Angshuman Nag
3	Mhatre Maitreyee Anant	Biodegradable polymer scaffolds for drug delivery	Dr. M. Jayakannan
4	Padmaja M.	Ruthenium-catalyzed highly regio-and stereoselective oxidative coupling of π-components : A versatile route to diense and heterocycles	Dr. M. Jeganmohan
5	Sarangamath	Functionalized nucleoside analogues for nucleic acid study by NMR and fluorescence spectroscopy	Dr. S. G. Srivatsan
6	Mallojjala Sharath Chandra	Organic sources of hydrogen sulphide	Dr. Harinath Chakrapani
7	Golu Parte	Synthesis of high surface area carbon materials and their functional composites with metal oxides for energy storage	Dr. Satishchandra Ogale, NCL Pune

Sl. No.	Name of the Student	Thesis Title	Thesis Supervisor
8	Sujoy Saha	Anion substitution in metal sulfides and selenides	Prof. C. N. R. Rao, JNCASR, Bangalore
9	Arya Thampi	Label-free imaging of intact, pigmented melanocytes	Dr. Mrinalini Puranik
10	Manish Kumar	Supramolecular chemistry of modified Tripyrranes	Dr. V. G. Anand
11	Nikhil Y. L. K.	Exploration of oxidation reactions using heterogenized Fe complexes under flow	Dr. Sayam Sengupta, NCL
12	T. Sriharsha	Nanoscale heterostructure interfaces for water splitting	Dr. Aninda J Bhattacharyya, IISC Bangalore
13	Raju Lunkad	Influence of concentrations on phase transformation of surfactant bilayers	Dr. Ananya Debnath, IIT Jodhpur
14	Pratyush Kumar Mishra	Development of fluorescent probes for hydrogen sulfide sensing	Dr. Pinaki Talukdar
15	Maddala Bala Gopal	Plasmonic property of doped semiconductor nanocrystals for chemical sensing	Dr. Angshuman Nag
16	Divya Mahendran	Surface chemical modification of biomimetic materials	Dr. Ashish Vaidya, Unilever R&D, Bangalore
17	Niranjana Sreelal	Calcium carbonate crystallization on household surfaces from Hard water	Dr. Amitava Pramanik, Unilever R&D, Bangalore
18	Pooja Prasanthan T.	Kinetics of SLES degradation in acidic environment and its impact on phase behaviour	Dr. Jiji Kottukapally, Hindustan Unilever Research Centre, Bangalore
19	Farzeena C.	Measurement of surface and interfacial properties	Dr. Narayanan Subrahmaniam Hindustan Unilever Research Centre, Bangalore
20	Thameez Mohammed K.Y.	Stimuli responsive polysaccharide vesicles for targeted anticancer drug delivery	Dr. M. Jayakannan

National Eligibility Test (NET) qualification

Name	Rank	Category	Year
Rohit Kumar	106	UGC-JRF	2011
Abhinaw Kumar	32	LS	2011
Kumbhare Rohan Surendra	34	CSIR-JRF	2012
Ankita Malik	44	CSIR-JRF	2012
Sreejith Varma.J	58	CSIR-JRF	2012
Akula Venumadhav	77		2012
Iti Kapoor	78	CSIR-JRF	2012
Rajkumar	81		2012
Veena Jessy	114	CSIR-JRF	2012
Monika Dash			2013
Anurag Agrawal			2013
Akula Venumadhav			2013
Rajkumar Yadav			2013
Pilli Veena			2013

BS-MS Students on Exchange Program for Summer Internship

Name	Exchange Program	University/Advisor	Year	Project Title
Upendra Singh	DAAD-WISE	Friedrich Alexander Universitat, Erlangen Nurnberg Advisor: Prof. Hans Peter Stienruck	2013	Reactions of 5, 10, 15, 20-tetraphenylporphyrin (2HTPP) molecules on Cu(111)
Meghana Raghunandan	FUB-INSPIRE (DST and Freie Universität, Berlin)	Freie Universität, Berlin Advisor: Priv.-Doz. Dr. Axel Pelster	2013	Spin orbit coupling in Bose-Einstein condensates
Sharad Joshi	UKIERI	University of Surrey Advisor: Prof. Ben Murdin	2013	Laser interaction with a 3 level system
Amey Anant Apte	UKIERI	University of Surrey Advisor: Prof. S. Ravi P Silva	2013	Fabrication and study of optical properties of subwavelength hole arrays on silver thin films
Shada Arun Dixit Reddy	Pelotonia Fellowship	Ohio State University Advisor: Prof. Ching-Shih Chen	2013	Synthesis of in-house focused compound library for a Novel Integrin-Linked Kinase Inhibitor
Monica Dash		CERN, Geneva, Switzerland Advisor: Joao Martins Guilherme Correia	2013	Use of Perturbed Angular Correlation (PAC) spectroscopy to optimize cleaning of polluted waters of heavy metal ions using specifically functionalized magnetite nanoparticles
Anurag Agarwal	DAAD-WISE	University of Gottingen Advisor: Prof. Ulf Diederichsen	2012	Inclusion of β -peptides to lipid bimembrane
Soumitra Athavale	DAAD-WISE	University of Gottingen Advisor: Prof. Ulf Diederichsen	2012	Synthesis of spin labels
Rohit Chikaraddy		Notre dame Radiation Laboratory Advisor: Dr. Ireneusz Janik	2012	State of the art UV induced Resonance Raman Spectroscopy
Neha Agarwal	DAAD-WISE	University of Gottingen Advisor: Prof. Ulf Diederichsen	2011	Synthesis and Characterization of analogs of Triostin-A using solid phase synthesis

Name	Exchange Program	University/Advisor	Year	Project Title
Iti Kapoor	DAAD-WISE	University of Regensburg, Germany Advisor: Prof. Dr. David Diaz Diaz	2011	Delicate balance between gelation and crystallization in multicomponent systems
Haritha Rao	DAAD-WISE	Goethe Universitat, Germany	2010	
Abhinav Kumar	DAAD-WISE	Universitaet des Saarlandes, Saarbrucken	2010	

Alumni Affiliation of Graduated Class of BS-MS Students

Sr. No.	Name	Present Affiliation
Class of 2011		
1	Haritha Rao	PhD in Chemistry -Goettingen university, Germany
2	Prakhar Arora	Shell India Ltd, Bangalore
3	Vedant Pande	Shell India Ltd, Bangalore
4	Rakesh Gaur	PhD in Chemistry - IISER, Pune
5	Ashutosh Priyadarshi	Shell India Ltd, Bangalore
6	D. Pravarthana	Erasmus Mundus scholarship- UCBN, Caen, France- PhD in Physics
7	Varun Kumar Rishi	PhD-Chemistry -University of Florida
Class of 2012		
1	Sandeep Gupta	PhD in Chemistry, BARC, Mumbai
2	Dharmraj Robins Chourasia	Genex Patent Office, Pune
3	Rohit Kumar	MBA at Indian Institute of Management (IIM), Kozhikode
4	Neha Agrawal	PhD in Chemistry, Purdue Univ, Indiana, USA
5	Anuj Bisht	Hey Math, Chennai
6	Prashant Agrawal	MSc, Queen's University, Canada
7	Abhinaw Kumar	PhD in Chemistry, University of Utah, USA
Class of 2013		
1	Piyush Agrawal	PhD in Chemistry, UTH, Zurich
2	Sumeet Kumar Singh	Ph.D in Chemistry, Ben - Gurion University, Israel
3	Nishant Singh	Hey Math, Chennai
4	Shreyas Supekar	PhD in Chemistry, TU Munich
5	Amit Kumar	Internship, Shell India Ltd, Bangalore

Sr. No.	Name	Present Affiliation
6	Iti Kapoor	PhD in Chemistry, UIUC, USA
7	Kumbhare Rohan Surendra	Ph.D in Chemistry, University of Pittsburgh, USA
8	Uma Sridhar	PhD, University of Massachusetts, Amherst, USA
9	Gawali Suhas Shahaji	IIT, Bombay for project
Class of 2014		
1	Anurag Agrawal	PhD in Chemistry, University of Wisconsin, Madison, USA
2	Vikas Negi	PhD in Chemistry, Eindhoven University of Technology, Netherlands
3	Rohit Chikkaraddy	PhD in Chemistry, University of Pennsylvania, USA
4	Vikash Kumar	PhD in Chemistry, University of Massachusetts, Amherst, USA
5	Amrit Kumar	PhD in Chemistry, University of Limerick, Ireland
6	Shada Arun Dixith Reddy	PhD in Chemistry, Rutgers University, New Jersey
7	Sumit Bhatnagar	PhD in Chemistry, National University of Singapore
8	Pilli Veena	Shell Technology Centre, Bangalore
9	Digvijay Porwal	PhD in Chemistry, MPI, TU Berlin
10	Pramod Kumar	Opening coaching class
11	Akula Venumadhav	PhD in Chemistry, IIT Mumbai
12	Ankita Malik	PhD, Max Plank Institute of Colloids and Interfaces, Germany
13.	Bhaisare Rupal Dinesh	PhD in Chemistry, IISER-Pune

List of Publications by Undergraduate Chemistry Students

1) Bandyopadhyay, A.; Agrawal, N.; Mali, S. M.; Jadhav, S. V.; **Gopi, H. N**. Tin(II) Chloride Assisted Synthesis of *N*-protected γ-amino β-keto Esters Through Semipinacol Rearrangement, *Org. Biomol. Chem.* **2010**, *8*, 4855.

2) **Verma, S**.; Pravarthana, D. One-Pot Synthesis of Highly Monodispersed Ferrite Nanocrystals: Surface Characterization and Magnetic Properties, *Langmuir* **2011**, *27*, 13189-13197.

3) Pramod, P. S.; Katamura, C.; Chapaker, S.; Balasubramaniam, N.; **Jayakannan, M.** Dextran Vesicular Carriers for Dual Encapsulation of Hydrophilic and Hydrophobic Molecules and Delivery into Cells. *Biomacromolecules* **2012**, *13*, *3627-3640*.

4) Rao, H.; Tanpure A. A.; Sawant, A. A.; **Srivatsan, S. G.** Enzymatic Incorporation of an Azide-Modified UTP Analog into Oligoribonucleotides for Post-transcriptional Chemical Functionalization. *Nature Protocols* **2012,** *7*, 1097–1112**.**

5) Tanpure, A. A.; Patheja, P.; **Srivatsan, S. G.** Label-free Fluorescence Detection of the Depurination Activity

of Ribosome Inactivating Protein Toxins. *Chem. Commun.* **2012, *48*, 501–503**. ***Selected as a Hot Article for ChemComm.***

6) Rao, H.; Sawant, A. A.; Tanpure A. A.; **Srivatsan, S. G.** Post Transcriptional Chemical Functionalization of Azide-Modified **O**ligoribonucleotides by Bioorthogonal Click and Staudinger Reactions. *Chem. Commu.* **2012, *48*, 498–500**. ***Selected as a Hot Article for ChemComm and cover page article.***

7) Kand, D.; Mishra, P. K.; Saha, T.; Lahiri, M.; **Talukdar, P.** BODIPY Based Colorimetric Fluorescent Probe for Selective Thiophenol Detection: Theoretical and Experimental Studies. *Analyst* **2012,** *137*, 3921-3924.

8) Kand, D.; Kalle, A. M.; Varma, S. J.; **Talukdar, P.** A Chromenoquinoline-Based Fluorescent off-on Thiol Probe for Bioimaging. *Chem. Commun.* **2012,** *48*, 2722-2724.

9) Kishor, P.; Pimparkar, S.; Padmaja, M.; **Jeganmohan, M.** Ruthenium-catalyzed Regioselective Oxidative Coupling of Aromatic and Heteroaromatic Esters with Alkenes Under Open Atmosphere**.** *Chem Commun.* **2012,** *48*, 2030.

10) Kumar, S.; Pande, V.; **Das, A.** π-Hydrogen Bonding wins Over Conventional Hydrogen Bonding Interaction: A Jet-Cooled Study of Indole...Furan Heterodimer. *J. Phys. Chem. A* ***2012,*** *116,* 1368-1374.

11) Singh, H.**;** Balamurugan, A.; **Jayakannan, M**. Solid State Assemblies and Photophysical Characteristics of Linear and Bent-core π-Conjugated Oligophenylenevinylenes. *ACS Appl. Mater. Interfaces*. **2013**, *5*, 5578 – 5591.

12) Sridhar, U.**;** Pramod, P. S.; **Jayakannan, M.** Creation of Dextrin Vesicles and Their Loading-Delivering Capabilities. *RSC Advances* **2013,** *3*, 21237 – 21241.

13) Jadhav, S. V.; Singh, S. K.; Reja, R. M; **Gopi, H. N.** γ-Amino Acid Mutated α-coiled Coils as Mild Thermal Triggers for Liposome Delivery. *Chem Commun*. **2013,** *49*, 11065.

14) Jadhav, S. V.; Misra, R.; Singh, S. K.; **Gopi, H. N**. Efficient Access to Enantiopure γ^4-Residues with Proteinogenic Side Chains and Structural Investigation of γ^4-Asn and γ^4-Ser in Hybrid Peptide Helices. *Chem. Eur. J.* **2013**, *19*, 5955.

15) Mali, S. M.; Bhaisare, R. D; **Gopi, H. N**. Thioacids Mediated Selective and Mild *N*-Acylation of Amines. *J. Org. Chem.* **2013**, *78*, 5550.

16) Patil, S.; Patil, S.; Gawali, S.; Shende, S.; Jadhav, S.; **Basu, S.** Novel Self-Assembled Lithocholic Acid Nanoparticles for Drug Delivery in Cancer. *RSC Adv.* **2013***, 3,* 19760-19764.

17) Patil, S.; Gawali, S.; Patil, S.; **Basu, S.** Synthesis, Characterization and in Vitro Evaluation of Novel Vitamin D3 Nanoparticles as Versatile Platform for Drug Delivery in Cancer. *J. Mater. Chem. B* **2013,** *1*, 5742-5750.

18) Gupta, A. K.; Reddy S. A. D.; **Boomishankar, R.** Facile Formation of Stable Tris(imido)phosphate Trianions as its tri- and hexa-nuclear Pd(II) Complexes in Polar Solvents. *Inorg. Chem.* ***2013,*** *52, 7608-7614.*

19) Thampi, A.; Babu K.; **Verma S.** Large Scale Solvothermal Synthesis and a Strategy to Obtain Stable Langmuir–Blodgett Film of $CoFe_2O_4$ Nanoparticles. *Journal of Alloys and Compounds* **2013**, *564,* 143 –150.

20) Balamurugan, A.; Vikash Kumar; **Jayakannan, M**. Carboxylic Distilbene Fluorescent Polymer Chemosensor for Temperature, Metal-ion and Biomolecule, *Chem. Commun*. **2014,** *50*, 842-845.

21) Islam, M.; Tirukoti, N. D.; Nandi, S.; **Hotha, S.** Hypervalent Iodine Mediated Synthesis of *C*-2 *Deoxy* Glycosides and Amino Acid Glycoconjugates. *J. Org. Chem.* **2014,** *79*, 4470-4476.

22) Ganesh Kumar, M.; Thombare, V. J.; Bhaisare, R. D.; Adak. A.; **Gopi. H. N**. Synthesis of Tetrasubstituted Symmetrical Pyrazines from β-keto γ-amino Esters: A Mild Strategy for Self-dimerization of Peptides. *Eur. J. Org. Chem.* **2014** (*accepted*).

23) Mali, S.M.; Ganesh Kumar, M.; Katariya, M. M.; **Gopi, H. N**. HBTU Mediated 1-hydroxybenzotriazole (HOBt) Conjugate Addition: Synthesis and Stereochemical Analysis of β-benzotriazole *N*-oxide Substituted γ-amino Acids and Hybrid Peptides. *Org. Biomol. Chem.* **2014**, *12,* 8462.

24) Bandyopadhyay, A.; Malik, A.; Kumar, M. G.; **Gopi, H. N**. Exploring β-Hydroxy γ-Amino Acids (Statines) in the Design of Hybrid Peptide Foldamers. *Org. Lett.* **2014**, *16*, 294.

25) Sankar, R. K; Kumbhare, R. S.; Dharmaraja, A. T.; **Chakrapani, H.** A Phenacrylate Scaffold for Tunable Thiol Activation and Release *Chem. Commun.* **2014**, DOI: 10.1039/C4CC07343F

26) Dharmaraja, A. T.; Jain, C.; **Chakrapani, H.** Substituent Effects on Reactive Oxygen Species (ROS) Generation by Hydroquinones. *J. Org. Chem.* **2014**, *79*, 9413-9417.

27) Khodade, V. S.; Sharath Chandra, M.; Banerjee, A.; Lahiri, S.; Pulipeta, M.; Rangarajan, R.; **Chakrapani, H.** Bioreductively Activated Reactive Oxygen Species (ROS) Generators as MRSA Inhibitors *ACS Med. Chem. Lett.* **2014**, 5, 777-781.

28) Chauhan, D. P.; Varma, S. J.; Vijeta, A.; Banerjee, P.; **Talukdar, P.** A 1,3-amino group migration route to form acrylamidines. *Chem. Commun.* **2014,** *50*, 323-325.

29) Nagarkar, S. S.; Unni, S. M.; Sharma, A.; Kurungot, S.; **Ghosh, S. K.** Two-in-one: Inherent Anhydrous and Water-assisted High Proton Conduction in a 3D Metal-Organic Framework *Angew. Chem. Int. Ed.* **2014**, *53*, 2638-2642.

30) Chaudhari, A. K.; Sharma, A.; Mukherjee, S.; Joarder, B.; **Ghosh, S. K.** Capsule Voided Nanospace Confinement in a π-Stacked Supramolecular Organic Solid *CrystEngComm.* **2014**, *16*, 4691-4695. (Invited Article)

31) Manna, B.; Singh, S.; **Ghosh, S. K**. Guest Driven Structural Transformation Studies of a Luminescent Metal-Organic Framework *J. Chem. Sci.* **2014**, *126*, 1417-1422. (Invited Article)

32) Manna, B.; Singh, S.; Karmakar, A.; Desai, A. V.; **Ghosh, S. K.** Selective Anion Exchange and Tunable Luminescent Behaviors of MOF based Supramolecular Isomers. *Inorg. Chem.* **2014**, (Just accepted).

33) Srivastava, A. K.; Praveen Kumar, B.; Mahawar, I. K.; Divya, P.; Shalini, S.; Boomishankar, R. Anion Driven $[Cu^{II}L_2]_n$ Frameworks: Crystal Structures, Guest-Encapsulation, Dielectric, and Possible Ferroelectric Properties. ***Chem. Mater. 2014,*** *26, 3811-3817.*

34) Gupta, A. K.; Srivastava, A. K.; Mahawar, I. K.; Boomishankar, R. Discrete and Polymeric Cu(II) Complexes Derived from in Situ Generated Pyridyl-Functionalized Bis(amido)phosphate Ligands, $[PO_2(NHPy)_2]^-$. ***Cryst. Growth Des. 2014,*** *14, 1701-1709 (appeared as spotlight article).*

35) **Verma, S**.; Kumar, A.; Pravarthana, D.; Deshpande, A.; Ogale, S. B.; Yusuf, S. M. Off-Stoichiometric Nickel Cobaltite Nanoparticles: Thermal Stability, Magnetization, and Neutron Diffraction Studies. *J. Phys. Chem. C* **2014**, *118*, 16246-16254.

36) Kumar,V.; Sengupta, A.; Gavvala, K.; Koninti, R. K.; **Hazra, P**. Spectroscopic and Thermodynamic Insights into the Interaction between Proflavine and Human Telomeric G-Quadruplex DNA. *J. Phys. Chem. B* **2014**, *118*, 11090-11099.

37) Ramya K. R.; Kumar R.; **Venkatnathan A.** Energy and Spectral Characteristics of Hydrogen Occupied Pure and Tetrahydrofuran Doped Water Cages, *Comp. Theo. Chem.* **2014**, *28*, 1039.

38) Joshi, S.; Shukla A.; Katiyar H.; **Hazra A.;** Mahesh T. S. Estimating Franck-Condon factors using an NMR quantum processor. *Phys. Rev. A* **2014,** *90*, 022303.

Int. Ph.D. and Ph.D. Students Information Sheet

Integrated Ph.D. Students Total: 26

Ms. Anindita Adak (2011)
Mr. Santosh Kumar Singh (2011)
Ms. Sneha Banerjee (2012)
Ms. Hridya V.M. (2012)
Mr. Rahi Masoom Reja (2012)
Ms. Meghna Manae A. (2012)
Mr. Anish Rao (2013)
Mr. Bharat Tandon (2013)
Mr. Arunabha Sen (2014)
Ms. Bandana Kumari (2014)
Mr. Girish Singh Bisht (2014)
Mr. Kingshuk Roy (2014)
Ms. Konoya Das (2014)
Mr. Aamod Desai (2011)
Mr. Jerrin Thomas George (2012)
Ms. Nandi Aditi Chinmoy (2012)
Mr. Kulkarni Amogh Mahesh Chandra (2012)
Mr. Abhishek Swarnkar (2012)
Ms. Aditi Dixit (2013)
Ms. Mehak Malhotra (2013)
Ms. Shivani Sharma (2013)
Ms. Kriti Gupta (2014)
Mr. Omshanker Tiwari (2014)
Mr. Prashant Jain (2014)
Ms. Shalini Pandey (2014)
Mr. Vikash Kumar Ravi (2014)

Ph.D. Students Total: 146

2008

Mr. Anupam Bandyopadhyay
Mr. Amar R. Mohite
Mr. Prakash R. Sultane
Mr. Sandeep Jadhav
Ms. Mahima Goel
Mr. Sachitanand M. Mali

2009

Mr. Maroti Govindrao Pawar
Mr. Nitin Bansode
Mr. Anupam Sawant
Mr. Tullimilli Yadagiri Gopalkrishna
Mr. Vijay Kadam
Mr. Dnyaneshwar Kand
Ms. Smita Kashyap
Mr. Sumit Kumar
Mr. Abhigyan Sengupta
Mr. Satish Malwal
Mrs. Minal Sachin Pednekar

2010

Mr. A. Dharmaraja
Mr. Arun Tanpure
Mr. Biplab Joarder
Ms. Indu Kaul
Mr. Pramod P.S.
Mr. S. Anantharaj
Mr. Sanjog Nagarkar
Mr. Santosh Gadekar
Mr. Satheesh Ellipilli
Ms. Wilbee D.S.
Mr. Kiran Reddy Baddigam
Mr. Mothukuri Ganesh Kumar
Mr. Bapurao Surnar
Mr. Biplab Manna
Mr. Lakshmi Vr Babu Syamala
Ms. Kavita Sharma
Mr. Sharad Garud - Deshmukh

2011

Mr. Rohan Dattatray Yadav
Mr. Dinesh Pratapsinh Chauhan
Mr. Venkateswararao Boddu
Mr. Krishna Gavvala
Mr. Vinayak Shahaji Khodade
Mr. Ravikiran Cg.
Mr. Kishor Padala
Mr. Mandar Vinod Kulkarni
Ms. Sohini Sarkar
Mr. Sudeb Ghosh
Mr. Soumya Mukherjee
Mr. Santosh Panchal
Mr. Rakesh Gaur
Mr. Partha Pritam Patra
Mr. Anantkumar Srivastava
Mr. Avishek Karmakar
Mr. Maidul Islam
Mr. Siva Koti Sangabathuni
Mr. Hari Krishna Bavireddi
Mr. Sushil Benke
Ms. Arundhati Roy
Mr. Balu Navale
Mr. Pramod Sabale
Mr. Ranguwar Rajendra
Mr. Barun Dhara
Mr. Rajendra Aluri
Mr. Karnati Narasimha
Mr. Kundansingh Pardeshi
Mr. Tanmoy Saha

2012

Mr. K. Rajkumar
Mr. Mahesh Deshmukh
Mr. Yettapu Gurivi Reddy
Mr. Tushar Khopade
Mr. Mahesh Gudem
Mr. Mallu Chenna Reddy
Mr. N. Ashok
Mr. Sathish Dasari
Mr. Ashok Yadav
Mr. Avdhoot S Datar
Mr. Bijoyananda Mishra
Ms. Madhuri Gade
Mr. Sappati Subrahmanyam
Mr. Nandha Kumar
Mr. Naganath Yadav More
Mr. Trimbak Mete
Mr. Shahaji More
Mr. Reman Kumar Singh
Ms. Aparna Banerjee
Ms. Bhagyashree Kulkarni
Mr. Rajkumar Misra
Mr. Abhik Mallick
Mr. Praveen Kumar
Mr. Prabhakar Pawar
Ms. Sonashree Saxena
Mr. Plawan Kumar Jha
Ms. Shalini
Mr. Sandeep Kumar Palvai
Mr. Shyamapada Nandi
Mr. Sayan Mondal

2013

Mr. Shinde Sopan Valiba
Ms. Sudeshna Manna
Ms. Srilatha Arra
Mr. Jagadeeswararao Metikoti
Mr. Ravikumar G.
Mr. R. Manikandan
Mr. Debasis Saha
Ms. Himani Rawat
Ms. Kathewad Neha Vijay
Mr. Deshpande Nilesh Umakant
Mr. Partha Samanta
Mr. Rakesh Pant
Mr. Manoharan R.
Mr. Shiv Pal
Mr. G Shiva Shanker
Mr. Yashwant Kumar

2014

Mr. Anil Yadav
Mr. Chandramouli Ghosh
Mr. Chethan D.S.
Ms. Joshi Niharika Hemant
Mr. K. Veeresh
Mr. Mullangi Dinesh
Ms. Neha
Mr. Neralkar Mahesh Renukadas
Mr. Paithankar Harshad Vaijanath
Mr. Rajasekar P.
Mr. Roy Bibhisan
Mr. Satpathi Sagar
Ms. Shahila Muhammed
Ms. Shammi Rana
Mr. Vijayakanth T.
Mr. Warankar Avinash Manohar
Mr. Ashok Kumar B.
Mr. Ambhore Madan Digambar
Mr. Walunj Manisha Balasaheb
Mr. Shinde Rameshwar Sudhakar
Mr. Bhaisare Rupal Dinesh
Mr. Patil Sohan Dilip
Ms. Preeti Chauhan
Mr. Ajay Kumar Sharma Mohan M
Mr. Balamurugan S.
Mr. Bhandari Pavankumar Janardan
Mr. Manoj Kumar Gupta
Mr. Sanjit Dey
Mr. Bhingardve Pramod Prabhakar
Mr. Shinde Ganesh Punjaram
Mr. Nisal Rahul Rajendra
Mr. Wasim Jeelani Mir
Mr. Kamal Kumar Mishra
Mr. Prakash Prabhat
Mr. Bappa Ghosh

Ph.D. Degrees (Chemistry) Awarded

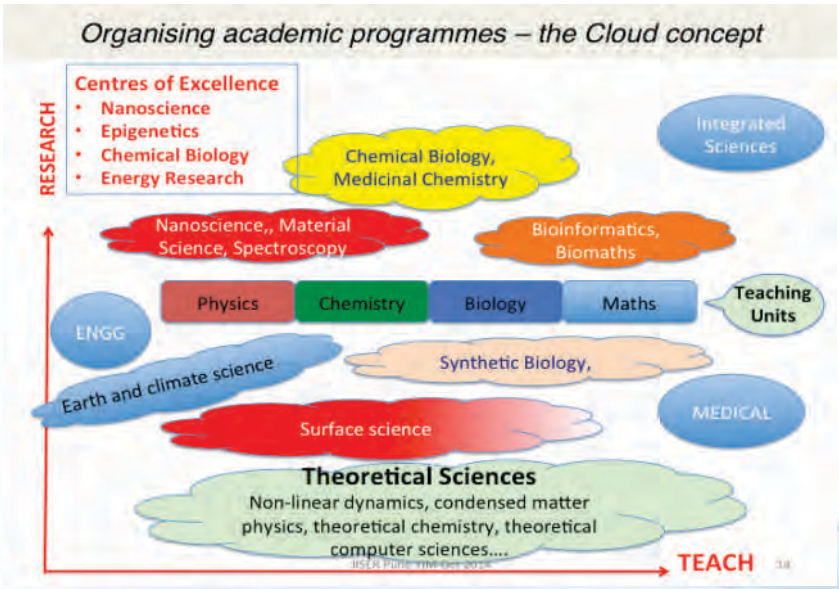
Sl. No.	Name	Title of Ph.D. Thesis	Thesis Supervisor	Ph.D. Degree Awarded	Present Affiliation
1	Dr. Anupam Bandyopadhyay	Synthesis and Utilization of Naturally Occurring Functionalized Gamma Amino Acids in the Design of Hybrid Peptide Foldamers	Dr. H. N. Gopi	2013	Post-doctoral Fellow, Boston College, Boston, USA
2	Dr. Mahima Goel	Supramolecular Assemblies of π-conjugated Phenylenevinylenes in Solid State	Dr. M. Jayakannan	2013	Lecturer, Department of Chemistry, Ramjas College, New Delhi
3	Dr. Amar R. Mohite	Atomistic Investigation of Polymer Electrolyte Membrane Nanostructure and Dynamics of Molecular Transport in Fuel Cells	Dr. R. G. Bhat	2014	Research Scientist, GVK Biosciences, Hyderabad (Pharma Company)
4	Dr. Sandip V. Jadhav	Design, Synthesis and Conformational Analysis of Hybrid γ-Peptide Foldamers Comprised of Proteinogenic Sidechains and Their Utilization in the Design of Novel Biomaterials	Dr. H. N. Gopi	2014	Post-doctoral Fellow, Institute of Bioengineering and Nanotechnology, Singapore

Sl. No.	Name	Title of Ph.D. Thesis	Thesis Supervisor	Ph.D. Degree Awarded	Present Affiliation
5	Dr. Sachitanand M. Mali	Chemistry on Unnatural Amino acid Peptide Building Blocks and Bioinspired Peptide Synthesis	Dr. H. N. Gopi	2014	Post-doctoral Fellow, Ben-Gurion University, Israel
6	Dr. Prakash R. Sultane	Total Synthesis of 1-Deoxy-6,7,8a-epi-Castanospermine, (+)-Epiquinamide, (+)-CP-99,994 and Orthogonal – Deacetylation and N-Cbz Deprotection	Dr. R. G. Bhat	2014	Research Scientist, TCG Life Sciences, Pune (Pharma Company)
7	Shivaji A. Thadke	Steroselective Glycosidations and Application to the Mycobacterial Arabinogalactand by Gold Catalysis	Dr. Srinivas Hotha	2014	Post-doctoral Fellow, Carnegie Mellon University, USA
8	Dr. Anurag P. Sunda	Atomistic Investigation of Polymer Electrolyte Membrane Nanostructure and Dynamics of Molecular Transport in Fuel Cells	Dr. Arun Venkatnathan	2014	Post-doctoral Fellow, JNCASR, Bengaluru
9	Dr. K. R. Ramya	Electronic Structure Characterization of Molecular Interactions in Clathrate Hydrates	Dr. Arun Venkatnathan	2014	Post-doctoral Fellow, University of Iceland, Iceland
10	Dr. Arvind Kumar Gupta	Synthesis and Functional Studies of Transition Metal Complexes Derived from Amino and Imido P(V) Ligands	Dr. R. Boomishankar	2014	Post-doctoral Fellow, National Dong-Hua University, Taiwan
11	Dr. Jain Deepak Ramesh	γ-C-Substituted Multifunctional Peptide Nucleic Acids: Design, Synthesis and Bioevaluation	Prof. K. N. Ganesh	2014	Post-doctoral Fellow, University of Boulder France
12	Dr. Abhigyan Sengupta	Excited State Dynamics and Photophysics in Bulk, Confined and Biomimetic Systems	Dr. Partha Hazra	2014	Post-doctoral Fellow, University of Colorado, Boulder
13	Dr. Sumit Kumar	Probing Non-covalent Interactions in Biomolecules and Materials: A Gas Phase Laser Spectroscopy Study of N-heterocyclic Aromatic Complexes	Dr. Aloke Das	2014	Post-doctoral Fellow, Max Planck Institute, Gottingen, Germany

Research & Development

The Chemical Sciences Department has 34 faculty, 150 Ph.D and 30 Integrated Ph.D. students, 20-25 MS students in their 5th year, actively pursuing research work in frontier areas of chemical sciences. The research areas fall broadly into 5 categoriesranging from chemical biology, computational chemistry, and spectroscopy to material science and catalysis.

The division has established two Centres of Excellence: (i) Nanosciences (funded by Nanoscience Initiative, from Department of Science and Technology, New Delhi) and (ii) Centre for Energy and Sustainable Environment (funded by the MHRD, Govt. of India, New Delhi). The division has also received support for high-end instrumentation (600 and 400 MHz NMR, spectrometer, X-ray diffractometer and Atomic Force Microscopy from DST, New Delhi under the FIST Level II Programme and is endowed with a number of advanced analytical equipments.



The thrust of the research programme in Chemistry at IISER Pune is motivated by cloud concept shown in the Figure above, with collaborative participation from faculty in other disciplines. It has active collaborations with various other research organizations in Pune such as CSIR-NCL, University of Pune and DRDO. Various international collaborations have been established through MoU signed at the Institute level, in particular with Goettingen University, Universities of Bath and Glasgow. The chemistry division at IISER Pune has emerged as one of the top 10 chemistry divisions in India. The research publications from the division have an average impact factor of 4.6 to 5.00/paper consecutively for the last four years.

The teaching programme has been recognized by the Royal Society of Chemistry (UK) through Accreditation in 2013. The faculties have received a number of peer recognitions such as Science medal of the Indian National Science Academy (Delhi), Young Associateship of Indian Academy of Sciences (Bangalore), medals from Chemical Research Society of India, Swarnajayanti Fellowship of DST etc. The following pages highlight research contributions from the Institute in the area of chemical sciences.

List of Faculty in Chemical Sciences

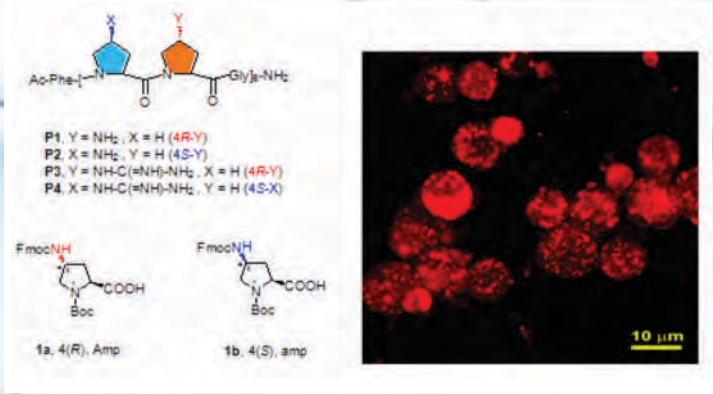
Name	Designation	Research
V. G. Anand	Associate Professor	Porphyrinoids, Molecular recognition, Luminescent materials
Nirmalya Ballav	Assistant Professor	Nanoscience, Self-Assembled Monolayers, Electron-Beam-Lithography, Molecular Spintronics
Ramakrishna G. Bhat	Associate Professor	Chemical biology, molecular mimicry, drug design, peptide and organic synthesis
R. Boomi Shankar	Associate Professor	Main Group and Organometallic Chemistry
S Sandanaraj Britto	Assistant Professor	Chemical Biology/Physiology & Optical Molecular Imaging of Whole Organisms
Harinath Chakrapani	Assistant Professor	Organic Chemistry, Drug Discovery, Nitric Oxide Prodrugs
Srabanti Chaudhury	Assistant Professor	Chemical physics, theoretical biophysics
Jeetender Chugh	Assistant Professor	NMR spectroscopy of biomolecules
Aloke Das	Associate Professor	Gas phase laser spectroscopy, Non-covalent interactions in biomolecules
Krishna N. Ganesh	Director, IISER Pune Professor and Coordinator	Biomolecular chemistry of nucleic acids, peptides, lipids; drug development, DNA diagnostics and nanotechnology
Prasenjit Ghosh	Assistant Professor	Atomistic modeling of Materials
Sujit K. Ghosh	Assistant Professor	Functional Coordination Chemistry, Organic-Inorganic Hybrid Materials, Supramolecular Chemistry
Boopathy Gnanaprakasam	Assistant Professor	Natural products synthesis, Asymmetric synthesis, Flow chemistry, Fluorination methods
Hosahudya N. Gopi	Associate Professor	Peptides and hybrid miniproteins, inhibitors for HIV-1 and host cell interactions
Anirban Hazra	Assistant Professor	Theoretical Chemistry
Partha Hazra	Associate Professor	Photophysics and biophysics
Srinivas Hotha	Associate Professor	Glycochemical Biology
M. Jayakannan	Associate Professor	Polymer chemistry and nano-materials
Jeet Kalia	Assistant Professor	Chemical Biology: Ion channels, lipids, and bioconjugation
Shabana Khan	Assistant Professor	Inorganic Chemistry
Raghavendra Kikkeri	Assistant Professor	Carbohydrates, Nanoparticles, Porous Silicon, Sialic acid and Glycomics
Jeganmohan M.	Assistant Professor	Organometallic chemistry, Asymmetric synthesis
B. S. Madhava Rao	Visiting Faculty	Pulse radiolysis, Time resolved spectroscopy, Fast kinetics
Moumita Majumdar	Assistant Professor	Main Group Chemistry-Catalysis and Materials Applications

Name	Designation	Research
Pankaj Mandal	Assistant Professor	Terahertz spectroscopy - applications to nanoscience and biomolecule dynamics
Arnab Mukherjee	Assistant Professor	Theoretical and computational chemistry, biophysics
Muhammed Musthafa	Assistant Professor	Interfacial Electrochemistry, Functionalized Surfaces, Energy Conversion and Storage Devices, Water Splitting, Sensors
A. A. Natu	Visiting Faculty	Organic chemistry, combinatorial chemistry, bio-organic chemistry, biology in drug discovery
Pramod Pillai	Assistant Professor	Functional nanomaterials: Hybrid nanostructures for self-assembly, light harvesting and bio-targeting studies
Mrinalini Puranik	Associate Professor	Biomolecular Spectroscopy, Raman spectroscopy of proteins, Nucleic acids
S. G. Srivatsan	Associate Professor	Chemical biology, nucleic acid chemistry, assay development, functionalised nucleic acids
Pinaki Talukdar	Assistant Professor	Supramolecular chemistry in lipid membranes, synthetic organic and medicinal chemistry
R. Vaidhyanathan	Assistant Professor	Metal organic frameworks for selective carbon dioxide sequestration
Arun Venkatnathan	Associate Professor	Molecular modelling, fuel cells and computational quantum chemistry
	Adjunct Faculty	
Sourav Pal	NCL, Pune	
	Faculty Fellows	
Dr. Angshuman Nag	Ramanujan Fellowship, DST, New Delhi	
Dr. Sudipta Basu	Ramalingaswami Fellowship, DBT, New Delhi	
Dr. Seema Verma	IISER Fellow, Pune	

A. Chemical Biology & Organic Chemistry

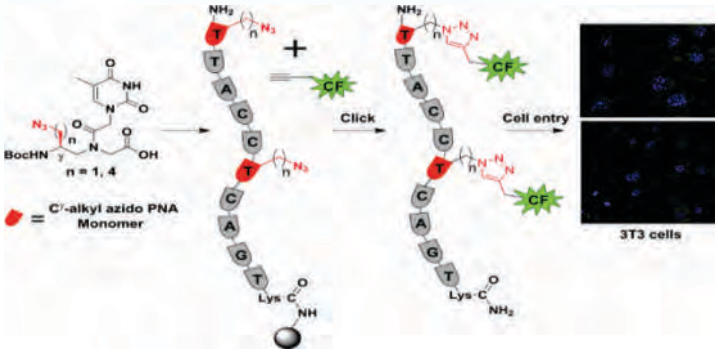
Peptides and Peptide Nucleic Acids

Intracellular drug delivery is a key component of contemporary drug development. Designing efficient mechanisms to deliver macromolecules, in particular, DNA and peptides to intracellular targets across impermeable cell membranes would create new therapeutic opportunities. Oligopeptides are attractive alternatives to cationic polymers and lipids for nonviral DNA delivery. Many cationic peptides induce translocation of DNA across the cellular membrane and deliver the attached cargo to the nucleus. In this context, proline-rich peptides have been shown to possess cell penetrating ability. The proline-rich collagen was found to transport plasmid DNA and siRNA into cells and



theoretical studies have supported formation of efficient DNA-collagen complexes. Previous work from this laboratory demonstrated a higher thermal and pH-dependent stability of 4(*R*/*S*)-aminoproline collagen peptides (**P1** and **P2**) compared to the analogous natural 4*R*-hydroxyproline peptides. The ionizable 4(*R*/*S*)-amino groups in these peptides are protonated at physiological pH making them cationic. Many cell penetrating peptides including polyprolines are cationic by virtue of having multiple arginine or lysine residues. The guanidium groups in proteins are known to recognise the anionic sulfate of heparin on the plasma membrane and translocate through cell membranes.

These observations prompted **Krishna Ganesh** and his group to fabricate the intrinsically cationic 4(*R*/*S*)-guanidinoproline collagen peptides **P3** and **P4.** The chimeric collagen peptides **P3** and **P4** were synthesized by 'on-resin" guanidinylation, and shown to efficiently transfect plasmid DNA having GFP reporter vector (pRmHa3-GFP) in S2 cells even in the absence of an *enhancer*. The fluorophere tagged 4-guanidinylproline cationic peptides are seen as punctuates in cell cytoplasm, localised in specific cytoplasmic organelles.

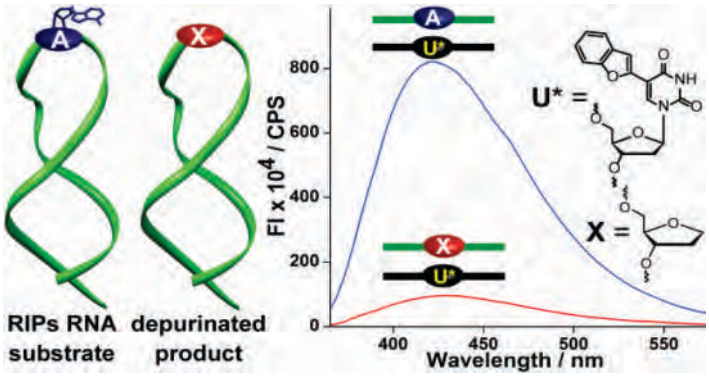


Other research work in **Krishna Ganesh**'s group is focused on the study of newer analogues of peptide nucleic acids, which are cell permeable and on investigating the secondary structures adopted by collagen type polypeptides, from a functional perspective. In the case of PNA analogues, the team has synthesized, characterized and studied the DNA complementation of clickable Cγ-substituted methylene (azm)/butylene (azb) azido PNAs. These analogues enhanced the stability of the derived PNA:DNA duplexes and fluorescent PNA oligomers synthesized by their click reaction with propyne carboxyfluorescein were seen to accumulate around the nuclear membrane in 3T3 cells.

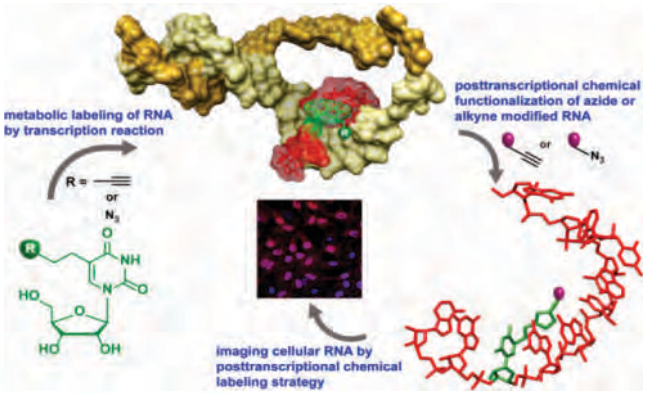
Extending this work to the corresponding Cγ-substituted alkylamino and guanidine PNA analogues, they have shown that these cationic PNA analogues are even better in stabilizing the cDNA/RNA sequences and permeate the cell more efficiently. Further, there was an asymmetric distribution in their localization around the nuclear membrane. Continuing their earlier work on (2S,4S)-aminoproline polypeptides, which showed β-structure specifically in trifluoroethanol, but not in water. They have now shown that the (2S,4S)-hydroxyproline polypeptides also exhibit similar behavior, confirming the importance of intra residue and inter chain H-bonding in dictating the formation of observed structures. Interestingly, the analogous (2R,4R)-hydroxyproline polypeptides showed a mirror image β-structure, which is hitherto unknown. These results have importance in designing new functional peptidomimetic systems.

Nucleic Acid Chemistry and Biophysics

Seergazhi G. Srivatsan' group is interested in developing tools to assess biological events by utilizing contemporary nucleic acid functions. In particular, his laboratory is interested in developing biophysical tools that would enable the study of nucleic acid structure, dynamics and function in vitro and in cells. He is also interested in developing multifunctional nucleolipid conjugates that could self-assemble into nanofibres, nanotubes and gels. It is expected that these self-assemblies would provide platforms for designing biosensors, biomaterials and scaffolds for non-templated/non-enzymatic oligomerization of nucleic acids.

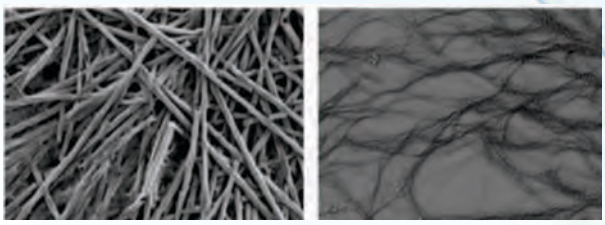


Functionalized nucleoside analogue probes: Nucleic acids perform a multitude of essential cellular functions such as storage and transfer of genetic information, catalysis and regulation of gene expression by interacting with nucleic acids, proteins and small molecule metabolites. **Srivatsan's** group has initiated a research program to develop structurally minimal perturbing and conformation-sensitive fluorescent nucleoside analogue probes for studying nucleic acid structure, dynamics and recognition properties in vitro and in cells. In particular, benzothiophene and benzofuran attached at the 5- and 8-position of pyrimidine and purine nucleosides, respectively, exhibited high fluorescence efficiency and excellent fluorescence solvatochromism. These analogues have been incorporated into RNA by enzymatic as well as chemical methods. His group has utilized them in developing fluorescence assays to (i) detect abasic sites (depurinated site) in DNA and RNA, (ii) monitor RNA-drug binding and (iii) study oligonucleotide dynamics in cell-like confined environment. Currently, his lab is developing multifunction nucleoside probes, which could be used to study the structure and function of nucleic acid simultaneously by fluorescence and NMR spectroscopy and by X-ray crystallography.



Chemical labeling and imaging of RNA: The Srivatsan group has recently developed a practical chemical labeling method for RNA by using novel toolbox made of azide- and alkyne-modified UTP analogues (*Nature Protocols* 2012, 7:1097, *Chem. Commun.*, 2012, 48:498). Some of these analogues are readily incorporated into transcribing RNA by endogenous RNA polymerases, which can be posttranscriptionally labeled with a variety of probes by bioorthogonal reactions such as click and Staudinger ligation reactions. The incorporation of azide-modified UTP analogue by endogenous RNA polymerases is the first example of selective labeling of cellular RNA transcripts with azide groups. The selective labeling of RNA with azide has enabled the group to devise a simple method to simultaneously image DNA and RNA synthesis in cells by using click reactions. It is expected that this modular and practical chemical labeling methodology will provide a new platform to study RNA in vitro and in cells (e.g., RNA synthesis, localization and degradation). His group is currently investigating the utility of this method in imaging RNA in live cells and animal models using fluorogenic probes.

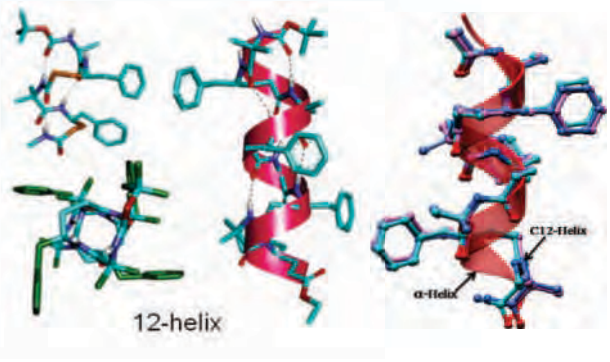
Functionalized nucleolipid conjugates: More recently, his group has designed, synthesized and studied the self-assembling properties of fluorescent nucleolipids made of new microenvironment-sensitive nucleoside (benzofuran- and benzothiphene-modified uracil) analogues as head groups and classical long chain hydrocarbons or fatty acids as lipophilic groups. These nucleobase- and nucleoside-lipid conjugates show self-assembling properties assisted by H-bonding, stacking and van der Waals interactions, and have been characterized by light microscopy, SEM, AFM and DLS methods. Currently, these self-assemblies are being utilized as platforms for designing biosensors, biomaterials and scaffolds for nontemplate oligomerization of nucleic acids.

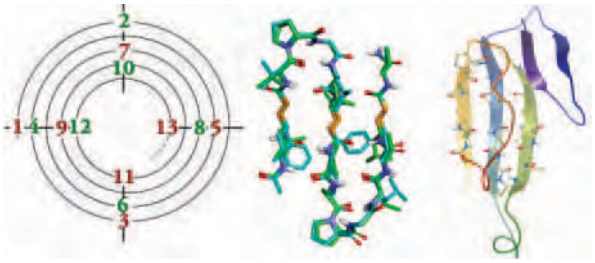


Peptidomimetics and Foldamers

Research in **Gopi's** group is mainly focusing on the exploration of naturally occurring non-ribosomal amino acids along with the novel α-, β- and γ-amino acids towards the design of proteolytically stable protein secondary structure mimetics, miniproteins, peptidomimetics and their utilization towards the structure based drug design for protein-protein interactions, protease inhibitors, antibiotics (antimicrobials), self-assembled soft biomaterials such as hydrogels, nanovesicles and nanotubes and exploitation of these soft biomaterials towards biology and material science.

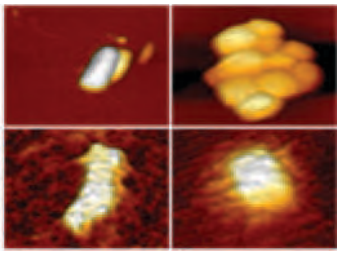
Foldamers: Designing synthetic protein structures using non-natural amino acids has immense importance from the perspective of medicinal chemistry. Significant progress has been achieved in this regard using the oligomers of β- and γ- amino acids and mixed sequences containing α/β and α/γ hybrid peptides. In contrast to the synthetic β- and saturated γ-amino acids, a variety of backbone functionalized γ-amino acids such as α, β-unsaturated γ-amino acids, β-keto-γ-amino acids and β-hydroxy γ-amino acids have been frequently found in many biologically active peptide natural products. In addition to their biological activities, these amino acids also provide a unique opportunity to exploit their functional groups for further derivatization. Inspired by the nature's selection, Gopi's group is exploring the utilization of these naturally occurring γ-amino acids along with the α-amino acids to design protein secondary structure mimetics and foldamers. Using these amino acids, various secondary and supersecondary structures such as β-sheets, β-hairpins, helices and multi strand β-sheets have been designed, synthesized and characterized in both solution and single crystals. The structural analogy of these novel hybrid peptides were assessed with the α- and β-peptides.

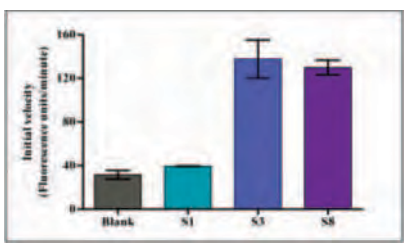




Gopi's group is presently investigating the α, γ-hybrid peptide helices designed using helical wheel diagram as inhibitors against the HIV-1 gp41 fusion process as well as P53-hDM2 interactions. The success of this strategy will be further explored for other protein-protein interactions.

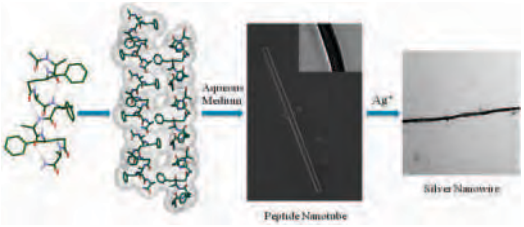
Anti-microbial properties and Mechanism of action of α, γ-hybrid peptides: Responding to the emergence of antibiotic resistant infectious microbes, Gopi's group is exploring proteolytically stable α, γ-hybrid peptides as potential anti-microbial candidates. By taking the guidance from natural anti-microbial peptides (AMPs), **Gopi's** group has designed short α, γ-hybrid lipopeptides and evaluated their anti-microbial activities. These short hybrid lipopeptides displayed broad spectrum anti-microbial properties against various bacterial and fungal strains. The mode of action reveals that they bind to the negatively charged outer membrane of the microorganisms and affecting the transmembrane electric potential. Inspired by the broad spectrum anti-microbial properties of short hybrid lipopeptides composed of *E*-vinylogous amino acids, Gopi's group is currently, investigating the anti-microbial activities of various short α,γ-hybrid lipopeptides, amphiphilic α,γ-hybrid peptide 12-helices designed from the helical wheel as well as „-hybrid peptide mixed 10/12 helices.

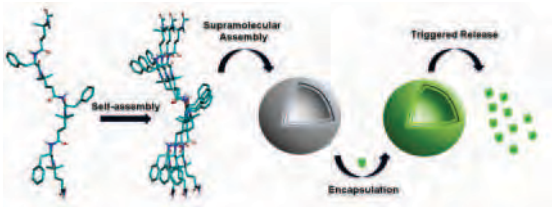


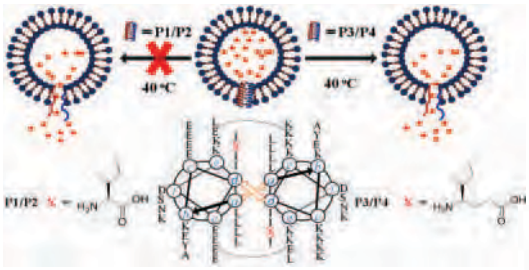


Biomaterials from hybrid peptides: **Gopi's** group is investigating the influence of amino acid side-chains and conformational rigidity of proteolytically stable hybrid peptides in the supramolecular assembly. Recently, they showed that designed hybrid peptide 12-helices with aromatic -amino acids hierarchically assembled into elongated nanotubes in aqueous environment. These nanotubes were further exploited in casting silver nanowires from silver ions. In addition, they also showed the spontaneous self-assembly of conformationally biased ,-hybrid peptides into stimuli responsive vesicles.

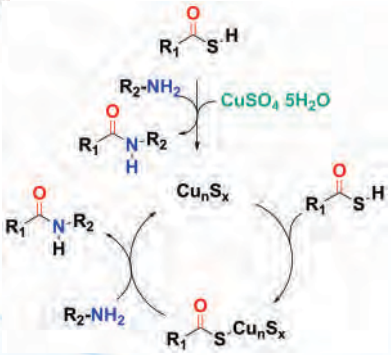
Further, **Gopi's group** has also reported the -amino acid mutated complimentary coiled-coil peptides as mild temperature triggers to release encapsulated molecules from the liposome-coiled-coil nanocomposites. Gopi's group is currently exploring these soft biomaterials as delivery vehicles, hydrogels for tissue engineering and casting metal nanowires for nanodevices.





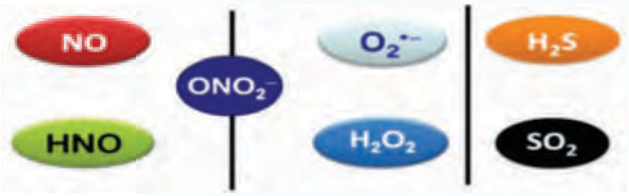


Developing strategies towards coupling agents free peptide synthesis: Gopi's group is also involved in developing new strategies for peptide synthesis.

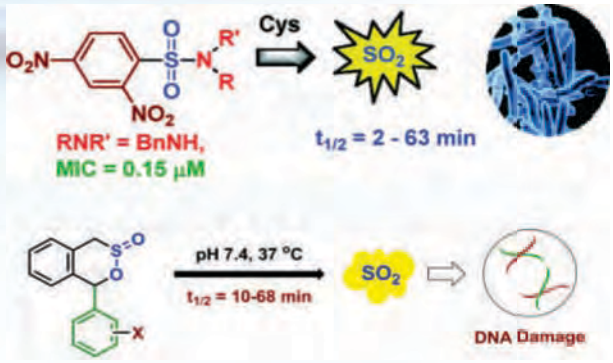


Chemistry and Biology of Reactive Species

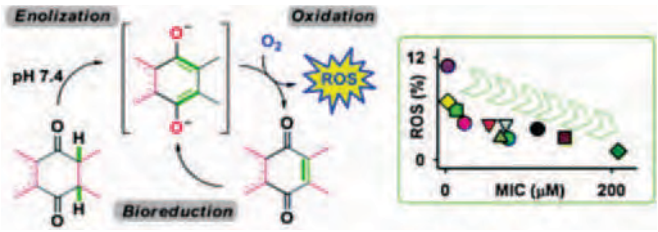
Nitrogen, oxygen and sulfur are elements that are indispensible for life as we know it. These elements exist in various oxidation states and nearly each of these redox forms has important physiological roles. Some examples are nitric oxide (NO), superoxide radical anion, hydrogen sulfide (H_2S) and sulfur dioxide (SO_2). These molecules share characteristics such as: being produced within cells; being gaseous, reactive and short lived; and causing macromolecular damage at elevated concentrations. However, biological studies that need to be conducted with such species require the use of precursors as the gases themselves are cumbersome to use. Tremendous progress in the understanding of the biological effects of nitric oxide is in part attributable to the availability of a large number of precursors of nitric oxide. However, the number of reliable surrogates for the other gaseous members of this class is few.



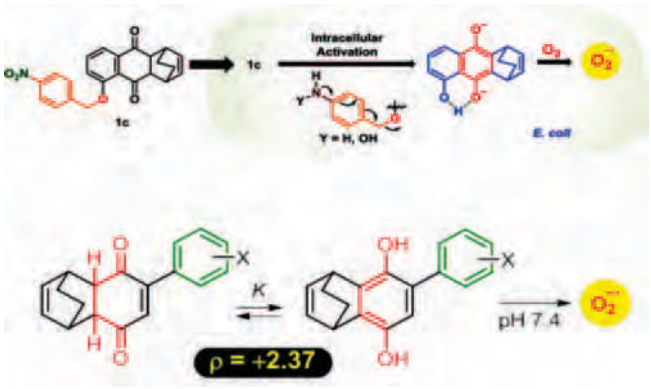
Harinath Chakrapani is designing and synthesizing organic compounds that can serve as reliable surrogates of such physiologically relevant reactive species. His group has developed novel sources of sulfur dioxide with half-lives ranging from a few minutes to several hours. Sulfur dioxide also has been extensively used as an anti-bacterial agent. These properties of sulfur dioxide might be exploited to develop new therapeutic agents. Several compounds prepared in his laboratory have shown potency against *Mycobacterium tuberculosis* comparable with a clinically used agent, isoniazid. His group has also developed benzosultines as donors of sulfur dioxide with tuneable half-lives. These compounds might find applications as tools for molecular biology studies.



Nearly all organisms inadvertently produce superoxide O_2, by 1-electron transfer to oxygen during respiration. O_2 is subsequently converted to hydrogen peroxide H_2O_2, which through Fenton reaction generates the highly reactive OH. Together, these reactive oxygen species (ROS) can damage vital cellular components and are hence deployed by the immune system to counter infectious pathogens. Although studies into the relationship between ROS and bacteria have been studied for several decades, a clear picture has not emerged. For example, recent studies have shown that antibiotics exert their lethality through enhancement of ROS. Several recent studies have shown that ROS can sensitize infectious bacteria to clinical antibiotics suggesting the possible therapeutic utility for ROS. His group has developed a hydroquinone-based scaffold for controlled generation of ROS upon dissolution in buffer. These compounds were found to generate ROS reliably and in excellent yield. A number of these compounds were found to inhibit *Mycobacterium tuberculosis*.



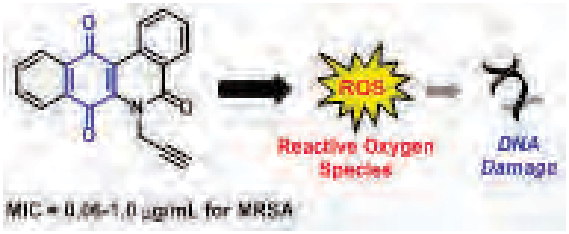
Using this scaffold, his group has also made an enzyme activated ROS generator. This small molecule generates ROS only when triggered by a bacterial enzyme and his group has demonstrated the capability of this compound to predictably enhance intracellular superoxide radical in a model bacterium. Spatiotemporal control over ROS generation offered by this compound should help better understand stress responses in bacteria to increased ROS.



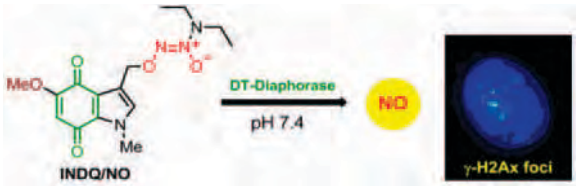
The structural aspects of the keto-enol equilibrium has also been studied by his group and they find that the propensity of hydroquinones to enolize determines ROS generating capability thus offering scope for tunable ROS generation.

Lastly, inspired by natural products, a library of phenanthridine-5,7,12(6H)-triones was prepared. A number of these compounds were found to undergo bioreduction to generate ROS. The group next tested the ability of these compounds to inhibit growth of the pathogen *Staphylococcus aureus* (*S. aureus*) and found several excellent inhibitors of this bacterium. This pathogen has acquired resistance to several antibiotics including the methicillin-based drugs. Methicillin-resistant *S. aureus* (MRSA) strains are fast becoming resistant to other frontline antibiotics as well. The group showed that the lead compound

generates reactive oxygen species (ROS) in the cell, contributing to its antibacterial activity. This compound was found to have potent *in vitro* growth inhibitory activity against numerous patient-derived clinical strains at levels comparable with Vancomycin, the drug of last resort for such infections.

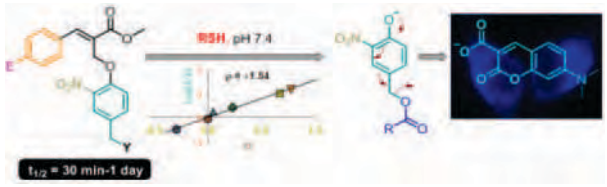


In addition, new strategies for site-directed delivery of nitric oxide via bioreductively-activated prodrugs and donors activated by hydrogen peroxide have been developed. Bioreductively activated NO donors were found to have excellent cancer growth inhibitory activity. The possible applications including using these NO donors as tools to overcome drug resistance as well as targeting hypoxic tumours is currently being explored.



Hydrogen peroxide activated NO donors present opportunities to study effects of NO during immune response. Both ROS and RNS are generated during immune response to counter infectious pathogens, presumably due to their ability to synergize leading to increased damaging effects. However, due to its antioxidant capability, NO has also been implicated in protecting bacteria from oxidative stress and may hence contribute to bacterial drug resistance.

In addition to developing new donors of reactive species, Harinath Chakrapani's group is also working on new prodrug activation methodologies. Recently, his group has developed a thiol-selective 2-methyl-3-phenacrylate scaffold with spatiotemporal control over delivery of a bioactive cargo. The half-lives of decomposition could be tuned from 30 min to 1 day and the scaffold's utility in thiol-inducible fluorophore release in cell-free as well as within cells was demonstrated.



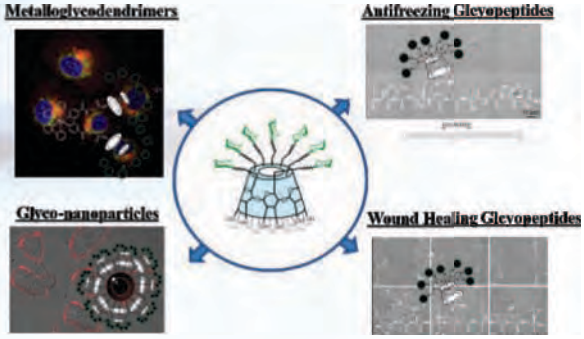
Glyco-nanobiotechnology

Carbohydrates play an important role in many biological systems by virtue of their lectins which recognize them. Carbohydrate-lectin interactions are involved in expansively diverse biological processes which include embryonic development, intracellular trafficking, cell-cell recognition, cell activation, cell adhesion, cell homing, endocytosis, phagocytosis, inflammation, tumor cell metastasis, and apoptosis. One main drawback for investigating carbohydrate-lectin interactions is their weak affinity to bind, which will require enhanced tools to analyze carbohydrate-lectin interplay. So far, two promising strategies have emerged from our studies: (1) designing multivalent glyco-probes using cyclodextrin templates and their utilization towards amplifying carbohydrate mediated targeting, self-assembly, and remote actuation of particles to treat tumors in cancer models and (2) developing biomimetic carbohydrate strategies to modulate carbohydrate-protein interactions.

Designing multivalent glyco-probes using cyclodextrin templates and their utilization towards amplifying carbohydrate mediated targeting, self-assembly, and remote actuation of particles to treat tumors in cancer models.

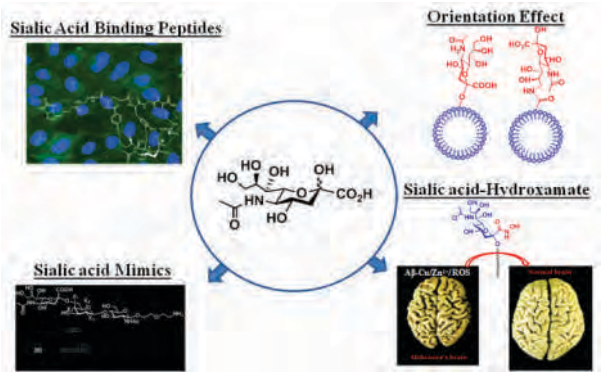
Designing multivalent template structures have immense importance not only to amplify the carbohydrate-protein interactions but also from the perspective of translational chemistry. Significant progress has been achieved in this regard using glyconanoparticles, glycodendrimers and glycopolymers. However, other important issues regarding the preparation of multivalent carbohydrates are related to the orientation, spacing and local concentration of the carbohydrates with respect to external stimuli. Therefore, it is important to form a general scaffold which is facile,

robust, presents tuneable symmetry and exhibits optical and electrochemical properties to develop a direct probing system. Inspired by the large number of supramolecular assembly of adamantoyl/β-cyclodextrin associated complexes, Dr. Raghavendra Kikkeri's group explored poly-glycosyl *β*-cyclodextrin probes in the synthesis of glyconanoparticles, metallo-glycodenderimers, photo-tuneable glycoclusters, glycopeptides, and glycoproteins. Using the multivalent nature of *β*-cyclodextrin, high-throughput microarrays and diagnostic kits were designed. Finally, *β*-cyclodextrins were expressed on cell surfaces using bio-orthogonal reaction to tune the behaviour and localization of cells. Currently, work on *β*-cyclodextrin-mediated remote actuation of particles to treat tumors is in progress.



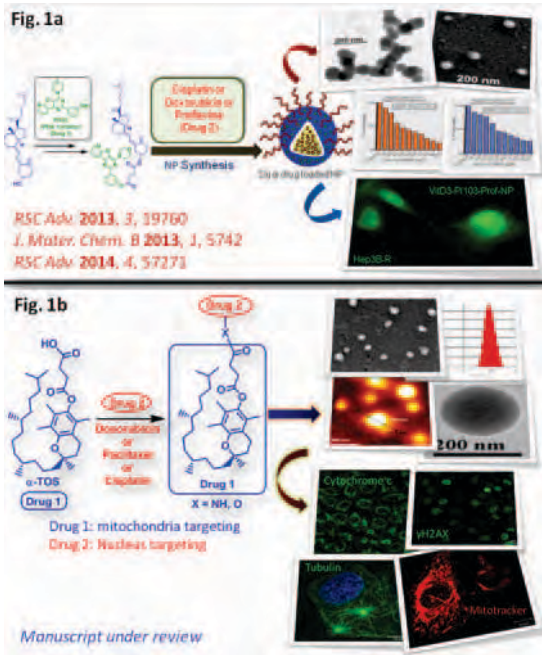
Biomimetic carbohydrates to modulate carbohydrate-protein interactions

Glycan-lectin interactions are important events in glycobiology. Numerous glycans have been synthesised and specific lectin interactions with many of these synthetic tools have been established. Despite the availability of a wide range of monosaccharide substrates, particular lectin mediated interactions require other tools such as multivalent carbohydrate displays or glycoprotein conjugation to improve binding. Recently, biomimetic syntheses of glycans are gaining momentum, primarily due to the ease in which one can synthesize a variety of novel glycans that may selectively enhance biomolecular interactions compared to natural ligands. As a prototype, **Kikkeri group** designed and synthesized a library of sialyl-mimetic glycans, which are known to bind a large pool of lectins such as C-type and I-type lectins. They anticipate that these synthetic analogs will induce strong binding and high specificity within specific subsets of lectins. Currently, the group is investigating carbohydrate-protein interactions and their potential applications as inhibitors and/or as promoters in specific biological recognition processes.



Chemical Nanobiotechnology

Cancer is one of the most devastating diseases in the world. Traditional cancer therapy uses highly cytotoxic drugs as chemotherapy alone or in combination with radiation therapy. However, most tumors can bypass the effect of monotherapy by developing intrinsic or acquired resistance mechanisms. Intrinsic resistance mechanism can pre-exist in the tumor through activation of redundant signalling pathways or overexpressing drug efflux pumps or mutational activation of downstream signalling. On the other hand, acquired resistance can develop during the treatment of tumor by mutations of the target or upregulation of other signalling pathways or downregulation of tumor suppressor proteins. It is now increasingly clear that none of these resistance developing



signaling pathways operate in isolation. Instead, each is influenced by crosstalk with other pathways. Moreover, complex positive- and negative-feedback loops serve to amplify or damp the signal fluxing through each of these pathways. As a result, signals (extracellular or intracellular) propagate through a tangled network of interconnecting organelles and cascades rather than through independent linear route. Hence to overcome this drug resistance in cancer **Sudipta Basu's group** proposes mechanism driven targeting of multiple organelles and multiple signaling hubs by merging chemical biology and nanotechnology to develop *chemical nanobiotechonology* tools.

Targeting multiple signalling pathways to overcome drug resistance: Rational combinatorial polypharmacy has emerged as an interesting strategy to target cancer drug resistance in the post-genomic era. However, The foremost shortcoming of current cancer chemotherapy is the diffusion of drug cocktails non-specifically leading to escalated toxicity of the drug combinations. Moreover, the drugs face the challenge to overcome biological barriers to reach the tumor target in right concentrations and combinations to offer effective therapeutic efficacy. To address these, Basu's group has developed a sub 200 nm particles from biocompatible, biodegradable vitamin D3 which can contain rational combination of dual drugs (PI103 and cisplatin or doxorubicin or proflavine) to target phosphatidyl-inositol-3-kinase (PI3K) signalling and DNA damage. The size, shape and morphology of these dual drug containing vitamin D3 nanoparticles were characterized by DLS, FESEM, AFM and TEM. The nanoparticles released the dual drugs in high quantity at pH = 5.5 compared to pH = 7.4 in a slow and sustained manner over 72h with stability over 15 days at 37°C as well as 4°C. These dual drug loaded nanoparticles induced increased cell death in human hepatocellular carcinoma, Hep3B cells at 24h compared to monotherapy; moreover, they were effective against cisplatin-resistant cells (Hep3B-R) as well. VitD3-PI103-CDDP-NP and vitD3-PI103-Dox-NP showed cytotoxicity by inducing apoptosis through DNA damage. Furthermore, vitD3-PI103-CDDP-NP showed much improved efficacy in 5-fluorouracil (5-FU) resistant Hep3B-5FU-R cells also compared to 5-FU. Finally, vitD3-PI103-Proflavine-NP internalized into the Hep3B-R cells much faster (within 3 minutes) compared to Hep3B cells visualized by fluorescent microscopy. Hence, these dual drug loaded nanoparticles can successfully overcome the trauma of drug resistance and has potential to be translated into the clinics for improved cancer therapeutics.

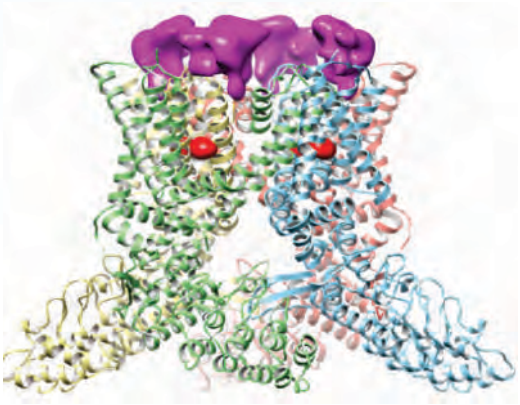
Targeting multiple organelles: In recent years, mitochondrion has emerged as an important alternative target in cancer therapeutics due to its diverse functions including cellular energy production by generating ATP via respiration, regulating danger signaling and containing mitochondrial DNA (mtDNA) as genomic material. Although, specific targeting of mitochondria emerged as an interesting strategy to alter the bioenergetics of cancer cells, mitochondria depend on the nucleus and other cellular organelles for most of their proteins and lipids as well as their cellular functions. The group hypothesize that nanoparticle mediated simultaneous subcellular targeting of mitochondria and nucleus would lead to more effective therapeutics in cancer. Aiming at this goal, They have chosen α-tocopherylsuccinate (α-TOS) as mitochondria targeting drug, cisplatin and doxorubicin as different clinically approved nucleus DNA damaging drugs and paclitaxel as microtubule binding drug to inhibit cell division. As a proof of concept the group has directly conjugated α-TOS with cisplatin, doxorubicin and paclitaxel without any additional linker. They engineered sub 200 nm particles from these dual drug conjugates which were endocytosed into the acidic lysosomal compartments of HeLa cervical cancer cells temporally and released the dual drugs in a slow and sustained manner to target mitochondria and nucleus simultaneously. These dual drug conjugated nanoparticles showed cytotoxicity by inducing apoptosis through damaging mitochondrial outer membrane (MOM) to release cytochome c as well as damaging nuclear DNA and tubulin to arrest the cell cycle. These dual drug conjugated nanoparticles have potential to simultaneous targeting of multiple subcellular organelles to escalate the therapeutic outcomes in modern cancer treatment.

Future direction: The Basu group has successfully demonstrated that nanoparticle mediated targeting of multiple signaling pathways can overcome drug resistance in cancer. Currently they are developing tools and techniques for organelle specific targeting of signaling pathways as well as targeting crosstalk between organelles to decipher their importance in disease state like cancer.

Chemical Biology: Ion Channels, Lipids, and Bioconjugation

There are three major focal points of interest of **Jeet Kalia's** chemical biology-centric research programme: ion channel biology, lipid biology, and bioconjugation. All projects in the laboratory are inherently interdisciplinary and combine disciplines as wide-ranging as electrophysiology, molecular biology, protein expression and purification, protein chemistry and organic synthesis.

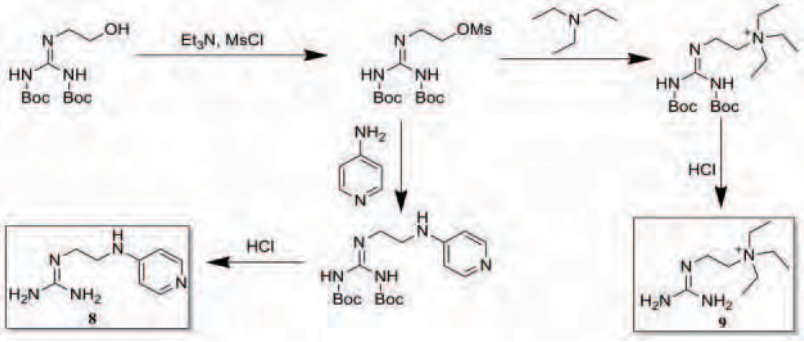
A major focus of research in the Kalia laboratory is to elucidate the molecular basis of how ion channel proteins open and close in response to stimuli such as voltage, temperature, chemical ligands and mechanical stress. These studies contribute to understanding how ion channel proteins endow organisms with vital life-sustaining traits such as cognition, pain-sensing, temperature-sensing and touch sensation. To achieve this goal, **Kalia's group** performs detailed structure-function based studies on ion channel proteins involving extensive site-directed mutagenesis of channels followed by the electrophysiological characterization of the resulting channel variants. Additionally, the group is developing specific small molecule and peptide modulators of ion channels that can be used as tools to elucidate the mechanism of ion channel gating and also may have therapeutic potential. For example, a recently published study by the Kalia group performed in collaboration with the Johns Hopkins and Emory Universities, resulted in the discovery of a novel anti-epileptic small molecule targeting voltage-activated sodium channels Nav1.1 modulation by a novel triazole compound attenuates epileptic seizures in rodents. *ACS Chem. Biol.* 9: 1204-1212). Moreover, the group has also contributed to a review on peptide toxins that modulate ion channel function.



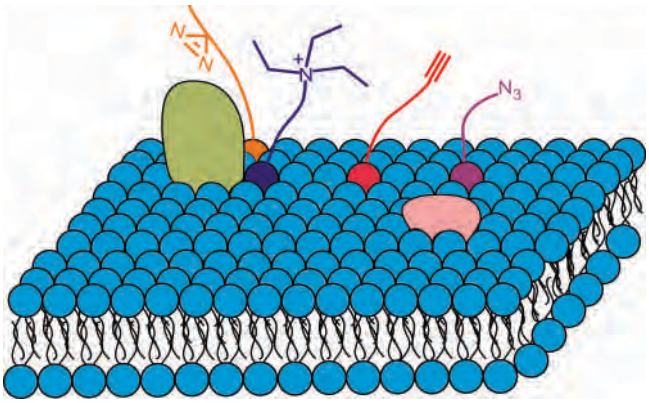
The Kalia laboratory is currently focusing on two projects on ion channels. One of these projects focuses on the Transient Receptor Potential (TRP) tetrameric cation channels that play important roles in several physiological processes such as temperature-sensing, mechanical stress-sensing and pain-sensing. The mechanistic underpinnings of how these channels are activated by such a diverse range of stimuli are extremely poorly understood. The recent discovery of a peptide toxin, the double-knot toxin (DkTx), produced by the Chinese bird spider, that specifically activates the TRP channel, TRPV1, has opened doors for the development of this toxin as a pharmacological tool for elucidating the gating mechanism of TRPV1 (Figure above). The Kalia laboratory has developed a high-yielding *E. coli* expression system for recombinant production of this toxin and is performing mechanistic investigations on DkTx-activation of TRPV1 by performing electrophysiological studies on channels expressed heterologously in *Xenopus laevis* oocytes and HEK293 mammalian cells.

Another ion channel-centric project in the laboratory focuses on the voltage-activated potassium (Kv) channels. Targeting Kv channels is a promising strategy for the therapy of multiple sclerosis and neuromuscular disorders such as botulism and Lambert-Eaton myasthenic syndrome. Indeed, the Kv channel inhibitor, 4-aminopyridine was recently approved by the Food and Drug Administration, U.S.A., for the treatment of multiple sclerosis. Additionally, the Kv channel-inhibitor, guanidine hydrochloride is sold as a prescription drug for the symptomatic treatment of Lambert-Eaton myasthenic syndrome. A major limitation of the therapeutic use of these compounds is the harmful side effects that accompany their administration. To overcome these detrimental side effects, the Kalia laboratory is designing analogs of aminopyridines and guanidines that may exhibit high potency for Kv channels, enabling administration at low dosage levels. Additionally, since the binding site of guanidine is adjacent but not identical to the binding sites of other Kv channel inhibitors such as tetraalkylamines and aminopyridines, compounds containing guanidine on one end, and aminopyridines or tetraalkylamines on the other end are also being synthesized (Scheme shown) in the hope of achieving potent Kv channel inhibtion.

In addition to ion channel biology, the Kalia research group is developing new approaches for studying the biology of lipids. In contrast to protein and nucleic acid research, lipid biology has lagged behind due to the lack of robust and



powerful tools to study lipids in cells. Unlike proteins, lipids are not genetically encoded, thereby precluding the use of genetics-based approaches that have revolutionized protein and nucleic acid biology. Modern mass spectrometry-based lipidomics has contributed significantly through precise estimation of the lipid compositions of cells. Nevertheless, mere quantification of lipid species is insufficient to elucidate their biological function. Rather, approaches for detailed *in vivo* functional studies of lipids are required. To address the urgent unmet requirement of tools for studying lipids in cells, the Kalia laboratory aims to employ metabolic labelling for the cellular incorporation of non-natural lipids that effectively mimic native lipids but have elaborated function (as shown in the Figure). These approaches will be utilized to incorporate lipid analogs in mammalian cells and *Xenopus laevis* oocytes which can serve as lipid "mutants" to interrogate the roles of lipids in membrane protein function. Such approaches will set the stage for applications in various other aspects of lipid and membrane biology such as the cell biology of lipids and membrane proteomics.



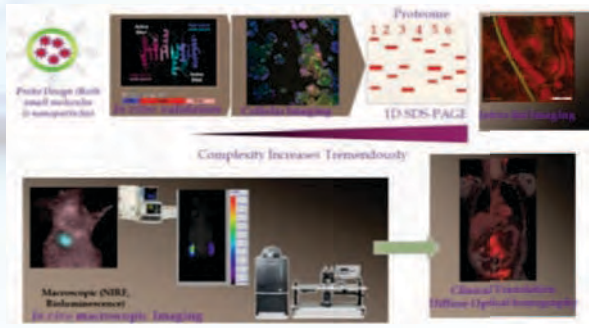
The third major focus of the Kalia laboratory is on bioconjugation. Recent breakthroughs in chemical biology have enabled the development of selective methods of covalently modifying proteins. These bioconjugation approaches have been utilized for a host of applications including imaging, disease diagnostic applications, and also for the discovery of interacting partners of protein(s) of interest in cells. Despite all this progress, two major limitations remain: 1) Several existing bioconjugation linkages are susceptible to hydrolysis and, 2) The rates of formation of bioconjugates are too slow to enable precise spatiotemporal applications in cells. To address these limitations, the Kalia laboratory is developing new methods of bioconjugation that proceed rapidly and result in stable linkages.

Chemical Physiology/Optical Molecular Imaging

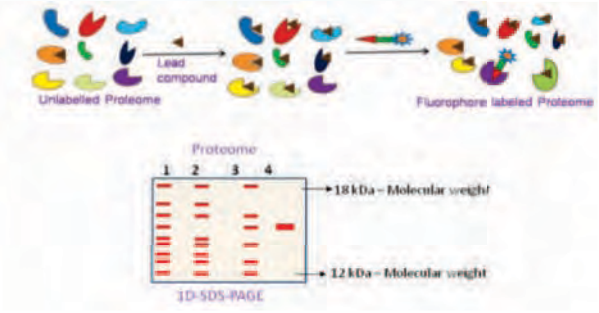
Britto's group research interest is designing new (macro) molecules for applications in the area of Chemical Biology/Physiology and Optical Molecular Imaging. In general, his research focuses on the following areas:

***In Vivo* Imaging of Enzyme Activity:** Enzymes are fundamental to all biological phenomena. Without enzyme-catalyzed biochemical reactions, no living forms can survive. No wonder, from development to differentiation, from metabolism to physiology and from cell division to cell death, all biological processes are dependent on the functions of "active" enzymes. In spite of decades of research on enzymes, in vivo monitoring of an enzyme function at single molecule resolution with very high substrate specificity is still a technical challenge. While enzymes have been studied at physiological concentrations and in both purified and in cell/tissue lysates, no technique is available to monitor the function of "active" enzymes in their native conditions in the milieu of all other components of living cells with very high resolution and exquisite specificity. Such studies will help us understand precise chemistry behind enzyme-substrate interactions and thereby to study regulation of complex biochemical reactions under various conditions. Technology to study enzyme function in vivo at very high temporal resolution and substrate specificity will have

immense application to understand diseases and also to test the efficiency of targeted drugs.



Activity-based Protein Profiling Technology: Standard genomic and proteomic technologies fail to address numerous post-translational forms of protein regulation controlling molecular and cellular function. Activity-based proteomics study addresses the limitations of standard genomic and proteomics methods. We are interested in developing new activity based probes for following applications: **(i)** Identification of novel drug targets; (ii) Determination of target selectivity of drug candidates in vitro, in cellule, ex vivo and in vivo (iii) Assessment of efficacy and toxicity for lead compounds & established drugs



Synthetic Virus Particles: Self-assembly of protein molecules to form beautiful nanostructures are exemplified in the nature by the presence of various types of viruses, which differ by their size and shape. Nature has worked its way through millions of years to come up with these aesthetic particles. Inspired by this, our group interest is to modify structure of globular proteins that would lead to self-assembly of protein molecules to make synthetic virus particle. The structure property relationship studies of this macromolecular entity should shed light on design principles of artificial virus particles.

Synthesis, Self-Assembly and Sensing

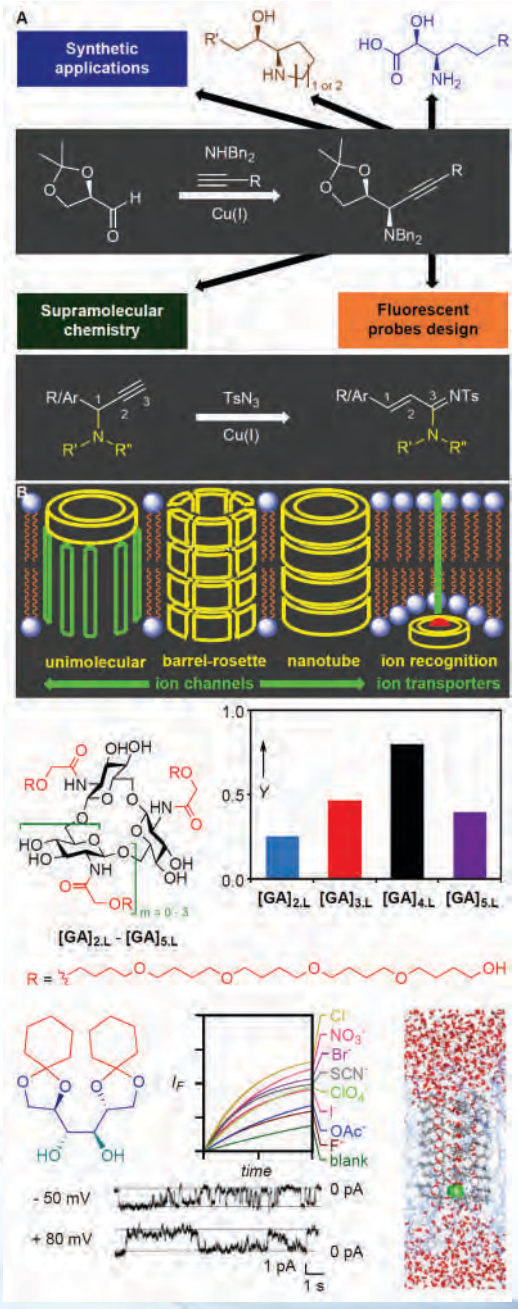
The research interest of **Pinaki Talukdar's** laboratory is to design of molecules for various functional applications. Targeted design of molecules is essential in diverse fields of research e.g. total synthesis, medicinal chemistry, chemical biology, supramolecular chemistry, etc. Present research of the laboratory covers areas synthesis, self-assembly and sensing. Under the sub area of synthetic chemistry, the research is focused in the development of synthetic methodologies. Further applications of these strategies are aimed in the synthesis of natural and non-natural product analogs. Beyond these, creation of molecules for supramolecular chemistry and sensing applications are also covered in the laboratory.

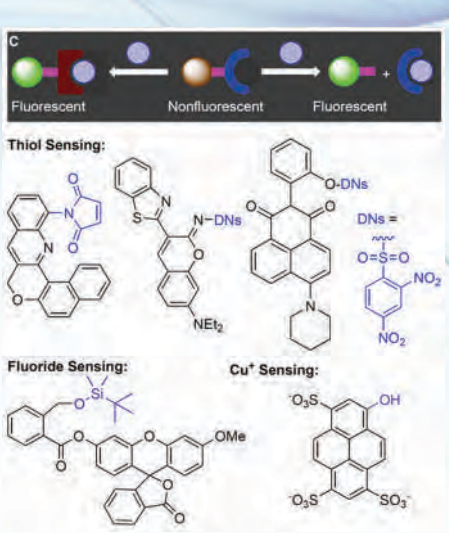
Recently, the Talukadar lab has exploited the Cu(I) catalyzed aldehyde-amine-alkyne coupling reaction as an efficient methodology for the construction of (2*S*,3*R*)-α-amino alcohol derivatives. Reactions of (*R*)-glyceraldehyde acetonide, dibenzylamine and terminal alkyne provided the amino alcohol with excellent diastereoselectivity. The methodology was applied further in the synthesis of various natural products and related libraries of molecules. Based on the methodology, they have carried out synthesis (+)-β-conhydrine, related pipiridine and pyrrolidine analogues. The utility of the methodology was also demonstrated by the stereoselective synthesis of valinoctin A and (2*S*,3*R*)-3-amino-2-hydroxydecanoic acid ((2*S*,3*R*)-AHDA). Another application of Cu(I) catalyzed reactions was addressed via the development of new reaction of the reactive ketenimine intermediate. In the presence of a tethered amino group, a 1,3-migration reaction was observed leading to the formation of acrylamidines. The group has also developed an enantiodivergent synthesis of both enantiomers of *δ*-unsaturated *γ*-amino acids. In the area of self-assembly, the group's research is focused in the development of ion channels and transporters. In recent times, they are working toward designs for artificial supramolecular ion channels and pores, and to mimic the functions their natural siblings. They have constructed unimolecular ion channels based on cyclo- oligo-glucosamines for tuning of ion transport activity. The group has also reported mannitol based rosette ion channels. These channels allow selective anion

transport via a hopping mechanism of ion from one rosette to the next. In the field of sensing, the research focus is on selective detection of species that are of either biological or environmental interests. These goals are addressed via the development of fluorescent probes. The Talukdar laboratory has developed diverse fluorescent probes for the sensing of thiols (*e.g.* biothols, aryl thiols, H_2S), anions (*e.g.* fluoride ion), cations (*e.g.* cations), etc. These probes are useful for rapid, selective and sensitive detection of respective analytes, and applicable for live cell imaging studies.

The future direction of the research will be focused in the fields of self-assembly and sensing. Various designs will be aimed in the design of functional supramolecules e.g. ion channels and transporters. One such strategy is proposed for modulating gating and selectivity of ion channels dictated by an external ligand. In 2000, Bayley and coworkers applied β-cyclodextrin derivatives as addapters for decreasing pore size of the α-hemolysin protein. Depending on the nature of the functional group attached to the β-cyclodextrin, the ion selectivity was also manipulated. We were encouraged by the strategy and propose to design synthetic ion channels which are expected to display gated opening by external ligands. The design will be focused to manipulate the ion selectivity by the nature of the external ligand. The second strategy in the supramolecular ion channels will be focused to construct stable nanotubular structures of different inner diameters. Based on the choice of monomer unit, the constructed nanotube will either allow the passage of only ions (inner diameter = 0.3 – 0.5 nm) or small molecules (inner diameter = 1.2 – 2.0 nm). This large nanotubular structure will be applied for molecular recognition studies, and carry out reactions in the confined environment. Therefore, based on the design, these self-assembled structures can function as either channel or pore in the transmembrane environment. Artificial ion channels will be studied for evaluating ion selectivity and results will be essential to understand fundamental knowledge on noncovalent interactions. The larger pore structures on the other hand, will be applied for sensing and delivery applications.

In the area of sensing, the group's aim will be focused in the design of cascade reaction based fluorescent probes. Such a strategy will be essential to address water solubility, membrane permeability, organelle specificity, reactivity and selectivity during sensing. In continuation with the group's recent work, goals are set to develop fluorescent probes for thiols (biothiols, H_2S, etc.), anions and metal ions of biological interests.





Chemistry of Saccharides

Hotha's research work is on development of methods for the chemical glycosylation and on their application into the synthesis of complex carbohydrate epitopes present on the cell surface of infectious microbes. Hotha's group is also focussed on the utility of *s*-tetrazine for the controlled synthesis of ternary and quaternary conjugates which will have a lot of ramifications. In yet another direction, Dr Hotha is also heavily involved in the making of TLC-MS interface machine and several new analytical instruments.

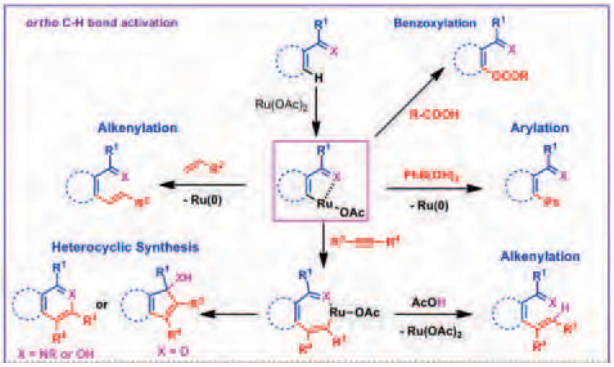
Non-invasive Diagnostics. Hotha's group is currently interested in the chemistry of furanosides wherein they have developed methods for the stereoselective synthesis of 1,2-*trans* and 1,2-*cis* furanoside by taking cues from the mycobacteriology. Quite recently, they have shown that less reactive glycosyl donors can be converted to more reactive glycosyl donors and Hotha's group showed its utility in the synthesis of arabinan present in the mycobacterial cell surface. Hotha and his co-workers are now trying to develop a diagnostic kit for the non-invasive detection of infectious bacteria in extra-pulmonary and CNS areas by exploiting glycolipid-glycolipid interactions.

Bioconjugation Methods. The utility of *s*-tetrazine for the synthesis of ternary conjugates by Hotha's group is one of the very first methods of their synthesis. *s*-Tetrazine offers differential SNAr reaction by the use of mercaptans and then the tetrazine nucleus can be subjected to the inverse electron demand Diels Alder reaction to get the ternary conjugates. Hotha showed that any combination of molecules can be subjected to this protocol and this approach is currently investigated in his group for probing co-operativity in lectin binding and protein-protein interactions.

TLC-MS Interface. Chemists use many tools for tracking the progress of reactions that they carry-out. One of the most versatile and ubiquitously used methods is the thin layer chromatography which is more popularly known as TLC. TLC examination gives the information on the progress of the reaction based on hydrophobicity of molecules and it does not give any kind of characterization data or confirmation about the chemical identity of the molecule of interest. Dr. Hotha and his team are currently developing an analytical tool which would give mass spectrum when coupled with a suitable mass spectrometer. The device will have two tubes out of which one takes the solvent from the reservoir and wets the sample of interest and the tube will then extract it from the TLC-plate and injects into the mass spectrometer. The necessary software and printed circuit board are developed and the probe head which actually houses both tubes is currently undergoing the fine tuning. The TLC-MS interface can also beused for obtaining samples directly from chromatographic plate so that the analyte can be subjected to other spectroscopic techniques as well. The device is named as ***S**oft**w**are **A**ssisted **D**irect **E**xtraction & **S**ampling **I**nterface (SWADESI).*

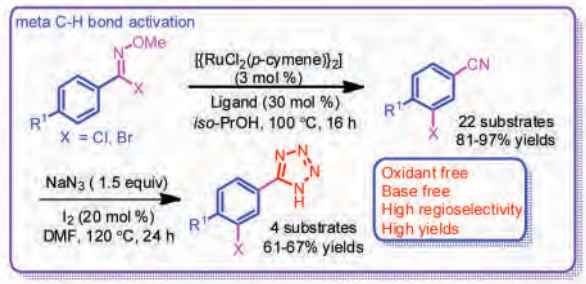
Metal Catalyzed C-H Bond Activation

The development of highly efficient, easily accessible and environmentally friendly method for constructing carbon-carbon and carbon-hetero bonds in a highly atom economical manner is highly important in organic synthesis. Metal-catalyzed reactions have been well-recognized as a powerful synthetic tool to construct carbon-carbon and carbon-hetero bonds in organic synthesis. M. Jeganmohan's group is mainly focused on the development of new synthetic methodologies by using transition metal complexes as catalysts in organic

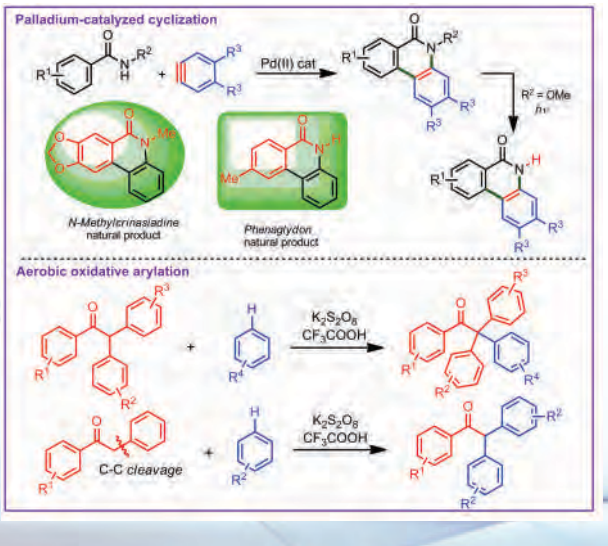


transformations. **Jeganmohan's group** is currently working on a ruthenium-catalyzed C-H functionalization of aromatics, heteroaromatics, alkenes and alkanes.

Construction of chemical bonds via metal-catalyzed chelation-assisted C-H bond activation of aromatics, heteroaromatics and alkenes followed by functionalization with nucleophiles or electrophiles is a powerful tool in organic synthesis. Palladium, rhodium and ruthenium complexes are widely used as catalysts in the C-H bond activation reaction. Among them, a less expensive ruthenium complex has gained tremendous attention recently, due to their remarkable reactivity, compatibility and selectivity. Interestingly, most of the ruthenium-catalyzed C-H bond activation reaction can be conducted under an air atmosphere. In 2011, Jeganmohan's group has demonstrated a ruthenium-catalyzed *ortho* alkenylation of aromatic and heteroaromatic ketones with olefins in a highly regio- and stereoselective manner. Later, this alkenylation reaction was successfully extended into aromatic aldehydes, esters and carbamates. In these reactions, 1,2-disubstituted alkenes were synthesized in a highly stereoselective manner. Later, his group has reported a ruthenium-catalyzed hydroarylation of aromatic carbamates with alkynes providing trisubstituted alkenes via a deprotonation metalation pathway. Further, the hydroarylation reaction was successfully extended with anilides and aromatic sulfoxides. Subsequently, his group has demonstrated a ruthenium-catalyzed *ortho* benzoxylation, acetoxylation and arylation of aromatic amides and anilides with organic carboxylic acids or aromatic and alkenyl boronic acids.



Apart from the *ortho* C-H bond activation, his group has described an unprecedented ruthenium-catalyzed intramolecular halogenation at the *meta* and *ortho* carbon position of *O*-methylbenzohydroximoyl halides under the base and oxidant free conditions in a highly regioselective manner.



In the meantime, his group has developed an efficient protocol to synthesize various heterocyclic molecules via a ruthenium-catalyzed oxidative cyclization of heteroatom substituted aromatics with carbon-carbon π-components. By employing this method, various heterocyclic molecules such as isocoumarins, indenols, isoquinolines, isoquinolones, α-pyrones, 2-quinolinones, isoindolinones and phenanthridinones can be prepared in good to excellent yields.

Subsequently, his group also demonstrated a metal-free aerobic oxidative dehydrogenative α-arylation at the sp^3 C-H bond of substituted ketones with aromatics or heteroaromatics in the presence of $K_2S_2O_8$ giving hindered symmetrical and unsymmetrical benzopinacolone derivatives under the mild reaction conditions. On the other hand, benzyl ketones reacted with aromatics providing α-diarylated ketones through carbon-carbon bond cleavage. The reaction was carried out at room temperature under an air atmosphere. In the reaction, two new carbon-carbon bonds were formed and one carbon-carbon bond was cleaved.

Jeganmohan's group has described various synthetic methodologies for synthesizing disubstituted alkenes, trisubstituted alkenes, halo substituted aromatic nitriles, *ortho* benzoxylated and arylated aromatics and heterocyclic molecules such as indenols, isocoumarins, fluorenones, substituted azoles, isoquinolones and isoquinolines. These methodologies would be very useful for synthesizing various natural products, biologically active molecules, polymers

and materials. In the near future, his group would like to focus on the *meta* selective C-H bond functionalization of aromatics and three component assembling of substituted aromatics with carbon-carbon π-components and electrophiles or nucleophiles via C-H bond activation in the presence of ruthenium catalysts. In the meantime, a proper effort will be devoted to synthesize biologically active molecules and natural products by employing his methodology as a key step and an enantioselective synthesis of organic molecules by using chiral ruthenium complexes as catalysts.

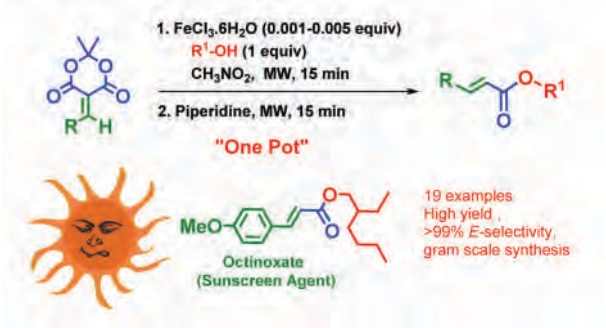
Strategies for Organic Synthesis and Catalysis

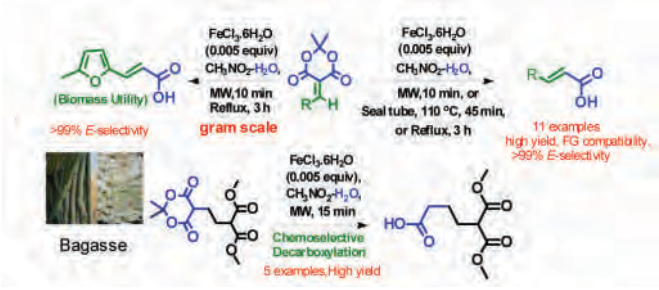
Ramakrishna G. Bhat's research group is involved in conducting research in the field of organic synthesis with a focus on green asymmetric catalytic synthesis and C-H functionalization, with an emphasis on the development of new synthetic methods that facilitate the construction of complex and bioactive molecules.

Recently, RGB research group has developed novel and practical protocols for the synthesis of cis-2,3-disubstituted piperidine derivatives, α,β-unsaturated acids/esters and useful strategy for N-deacetylation. (+)-(2S,3S)-CP-99,994 is a potent antagonist of substance P NK-1 receptor developed by Pfizer. Cis-2,3-stereochemistry is known to be very essential for this activity. Methods for introducing different substituents at C-2 at late stage have been very difficult and not well explored in the literature. Owing to the importance of the molecule, RGB group developed a very simple and efficient stereoselective approach to cis-2,3-disubstituted piperidines via the reduction of *N*-acyliminium ion intermediates. Starting from commercially available ornithine, corresponding amino ketones have been prepared using aryl magnesium bromides. Treatment of this with trimethylsily triflate and triethyl silane resulted in *cis*-2,3-disubstituted piperidines. Stereochemistry has been confirmed by using nOe studies and single crystal X-ray analysis. Application of this methodology has been exemplified by the enantioselective total synthesis of (+)-(2S,3S)-CP-99,994.

The α,*β*-unsaturated acids are very important and useful reagents in organic synthesis. These are significant structural motifs in many natural products (viz. the secretion of the queen honey bee, caffeic acid), pheromones and bioactive compounds. Similarly, α,*β*-unsaturated esters have been utilized as versatile building blocks in organic synthesis and find significant use in industry. Unsaturated esters such as cinnamate esters have been used as commercial sun screen filters. Most of the methods for the synthesis of α,*β*-unsaturated acids/esters are non-catalytic and less stereoselective. Environmentally benign and sustainable catalytic protocols with milder conditions which can tolerate a wide variety of functionality are highly desirable.

RGB research group developed a novel, practical and convenient catalytic protocol comprising $FeCl_3.6H_2O$ and H_2O (1 equiv) in CH_3NO_2 for the rapid synthesis of α, *β*-unsaturated carboxylic acids with high *E*-stereoselectivity both





under microwave and conventional heating conditions. This powerful approach efficiently demonstrated the utility of biomass derived aldehydes to build chemical agents as fuel additives. The method proved to be scalable to gram scale synthesis.

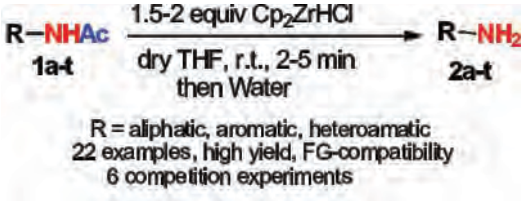
They explored for the first time controlled monoelectrophilic reactivity of alkylidene Meldrum's Acids with water using Lewis acid to synthesize α,β-unsaturated carboxylic acids with high stereoselectivity. *p*-Methoxycinnamates are commonly used as sunscreen chemical filters in industry and octyl methoxycinnamte (Octinoxate, OMC) is a common ingredient in most sunscreen lotions. This chemical, of commercial significance, has been the target of synthesis by various routes.

Having explored the synthesis of α,β-unsaturated carboxylic acids, the RGB research group has developed a facile and convenient synthesis of α,β-unsaturated esters by exploring the reactivity of alkylidene derivatives of Meldrum's Acid with different alcohols. Protocol uses a catalytic amount of $FeCl_3.6H_2O$ (0.001 – 0.005 equiv) with alcohols (1 equiv) in CH_3NO_2 followed by piperidine. A variety of α,β-unsaturated esters has been synthesized with high *E*-stereoselectivity in good to excellent yields.

The application of this methodology has been demonstrated by gram scale synthesis of octinoxate, a sunscreen agent, and other *p*-methoxy cinnamate esters. Reactions are neat and by-products formed are volatile. The novel protocol described for the selective esterification and decarboxylation uses very low catalyst loading (0.001 – 0.005 equiv, 0.1-0.5 mol%).This methodlogy provides an easy access to a range of α,β-unsaturated esters, including compounds of high industrial value, and on a gram scale.

Alongside, the RGB research group has been working on metal mediated strategies.

N-deacetylation usually needs harsher conditions and most of the reaction conditions are not suitable for sensitive substrates that are prone to racemization. A mild and efficient *N*-deacetylation using the Schwartz reagent at room temperature in rapid time has been developed (*Org. Biomol. Chem*. 2014, *12*, 261-264).



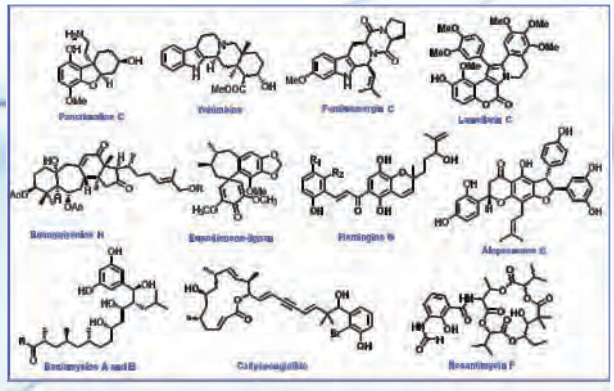
This *N*-deacetylation protocol is chemoselective and conditions did not induce any epimerization at chiral amino centre. Mild condition enables the orthogonal *N*-deacetylation in presence of some of the common protecting groups (*viz*. Boc, Fmoc, Cbz, Ts). The deprotection conditions did not induce any epimerization at chiral amino centre. Mild reaction condition, simple workup procedure provides a platform for the *N*-deacetylation without the use of any base or acid.

Currently the lab is focusing on the quinine/Cinchona catalyzed asymmetric reactions and thiourea derived organocatalysis. Thrust is on searching a) alternative catalysts, b) alternative synthetic strategies and methodologies for green asymmetric catalysis.

Similarly, novel reactions that can selectively functionalize C-H bonds are of great interest to the chemical community as they offer novel and efficient strategies for the organic synthesis. C-H functionalization is a very useful strategy and molecules can be modified at the late stage. RGB research group is concentrating their efforts on the metal carbenoid asymmetric intermolecular C-H functionalization using non toxic early transition metals/non-toxic metals at ambient conditions. Some of these strategies will be employed for the enantioselective synthesis of bioactive natural products and inhibitors of PI-3/Aurora Kinases and proteases in future.

Natural Products Synthesis and Catalysis

Natural products are benchmark for discovery of many drugs and currently one third of them are being used as drugs. Many steps involved in several classical total syntheses often make the synthetic routes economically unviable for industrial-scale processes. Synthetic organic chemists are therefore now using their *savoir faire* to invent short, practical



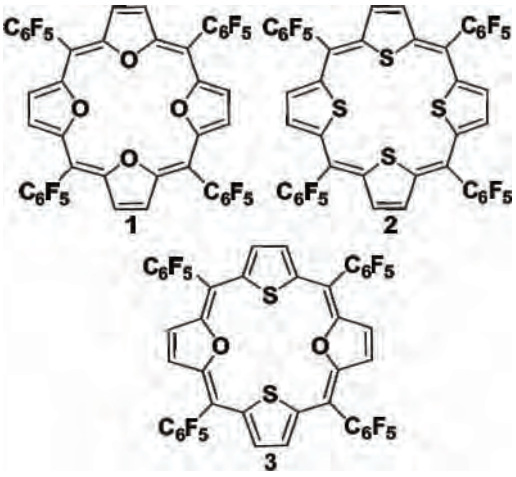
approach for natural-product syntheses with minimal impact on the environment.Therefore, the discovery of new catalytic reactions with sustainability is being required for the current synthetic processes.

Gnanaprakasam's research group is developing novel, efficient and sustainable route to synthesize natural products of challenging structures with intriguing biological activities. Towards these, his research group is focusing on developing new catalytic reactions using cooperative metal catalyst for stereoselective C-C, C-N and C-O bond formation by domino/tandem fashion or by dehydrogenates coupling methods to approach key building blocks in absence of hazardous stoichiometric reagents and activators without generation of any waste. **Gnanaprakasam**'s research group is also developing sustainable and efficient methods for the synthesis of chiral amines and bioactive heterocyclic compounds that are widely used in chemical industry and in natural products synthesis, via enantioselective amination by employing chiral cooperative metal catalyst. **Gnanaprakasam**'s research group is also exploring use of flow techniques for metal catalyzed organic transformations of industrial importance. Research on catalytic fluorination of various activated/non-activated aromatic and non-aromatic compounds using cooperative metal catalyst, non-hazardous and inexpensive fluorinating agents are also focused in his research groups.

B. Inorganic Chemistry, Catalysis and MOFs

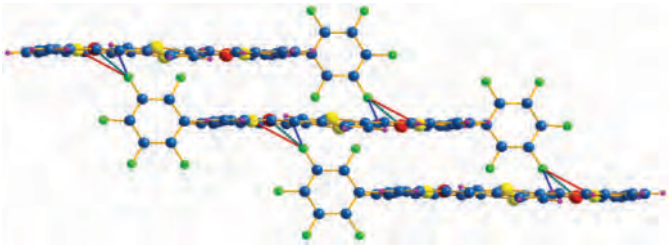
Macrocycles, Antiaromaticity and Noncovalent Interactions

V. G. Anand's research is focused on the synthesis of stable and novel antiaromatic macrocycles. Aromaticity and antiaromaticity are intriguing offshoots of π delocalization in cyclic conjugated systems. Their electronic effects and structural features are interdependent and crucial to conjugated macrocycles. 18π porphyrin and 20π isophlorin are striking examples of cyclic conjugated systems with structural features akin to annulenes and contrasting ring current effects. 4nπ macrocycles can react quickly to lose their antiaromatic character. The isophlorin-porphyrin redox couple further illustrates the unstable nature of isophlorin relative to porphyrin under ambient conditions. Interestingly, steric hindrance favor macrocycles to undergo structure induced loss of π delocalization. Giant porphyrinoids are well studied examples for macrocycles which adopt figure of eight conformations. Such non-planar cyclic conjugated systems lack ring current effects and are considered to be non-aromatic in nature. Relative to aromatic systems, the experimental evidence reported for antiaromaticity is found to be far less than satisfactory. There are very limited reports to bridge theoretical predictions with experimental data, particularly for large antiaromatic systems. In this context, synthesis of stable quintessential planar 4nπ molecules is crucial not only to understand the electronic effects of π conjugation but also imperative to the development of novel materials for applications in molecular electronics.



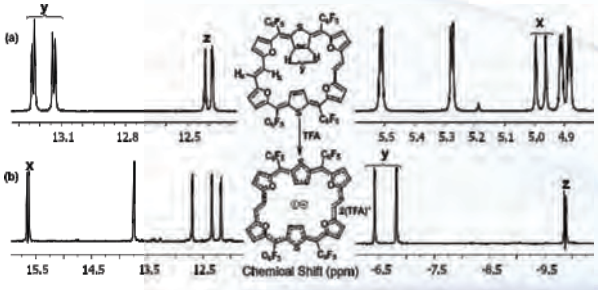
Isophlorin represents fused conjugated networks of annulene and porphyrin. It is derived either by reduction of a porphyrin copper complex or by two electron reduction of N,N',N'',N'''-tetramethyl-octaethylporphyrin dication. It

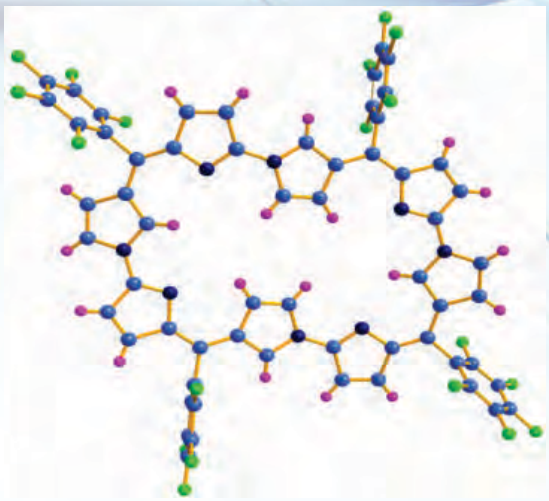
can rapidly transform itself into aromatic 18π system due to the fast conversion of two of its four cyclic amines to imines. Attempts to make isophlorin like macrocycles, have yielded only tetrathia/oxa/selena porphyrin dications (as their perchlorate salts). Vogel and co-workers were successful at characterization of tetraoxaisophlorin in solution state, but x-ray crystallographic analysis was less precise due to static and possible dynamic disorders. For the first time, synthesis, isolation and characterization of isophlorins as neutral and stable species was successfully achieved by V.G. Anand's group. The replacement of pyrrole rings by furan and thiophene have yielded three different types of stable 20π isophlorins 21,22,23,24-tetraoxaisophlorin (**1**), 21,22,23,24-tetrathiaisophlorin (**2**) and 21,23-dioxa-22,24-dithiaisophlorin (**3**). From ^{1}H NMR spectrum, it was observed that all the macrocycles were found to be anti aromatic in nature as expected of 4n system. Crystal structure analysis confirmed the planar structure for **1** and **3**, while **2** displays a non-planar structure due to steric crowding by four bulky sulfur atoms.



The π expansion of isophlorin like macrocycles by increasing the number of heterocyclic units yields stable 30π and 40π conjugated systems. These expanded systems show different structural features depending on the kind of heteroatoms at the core of the macrocycle. The group has been successful in the synthesis and characterization of 32π vinylogous expanded isophlorins using thiophene and selenophene as the building blocks for these cyclic systems. In this process they have developed a simple synthetic process by employing easy to make precursors under mild reaction conditions. Their electronic and structural properties confirm the antiaromatic nature both in solution and solid states. The most interesting fact about these systems pertain to very rare F…X (X = S/Se/π) interactions in the solid state, particularly for 4nπ systems. Their antiaromatic property has been confirmed by both experimental and computation studies. Our goal, now, is directed towards the possible role of electronic effects to affect such non-bonding interactions in antiaromatic systems.

Furthermore, for the first time, the group has shown redox dependent inter-changeable conformations for an expanded isophlorins. Spectroscopic analysis, single crystal X-ray diffraction studies and quantum chemical calculations reveal the formation of stable aromatic dications upon the addition of TFA, [$Et_3O^+SbCl_6^-$] or $NOBF_4$. In contrast to the generation of radicals from aromatic systems, [$Et_3O^+SbCl_6^-$] or $NOBF_4$, tend to oxidize antiaromatic systems to aromatic dicationic species. These dications can be reduced back to their neutral antiaromatic state by a variety of reducing agents such as zinc, $FeCl_2$ or triethyl amine. In spite of the apparent thermodynamic stability for aromaticity, reversible process between 4nπ and (4n+2)π states may be attributed to the facile reduction of aromatic dicationic species towards neutral antiaromatic state. This represents a prime example of an antiaromatic isophlorinoid and its corresponding aromatic dication as a reversible couple to inter-convert amongst themselves with suitable redox reagents.

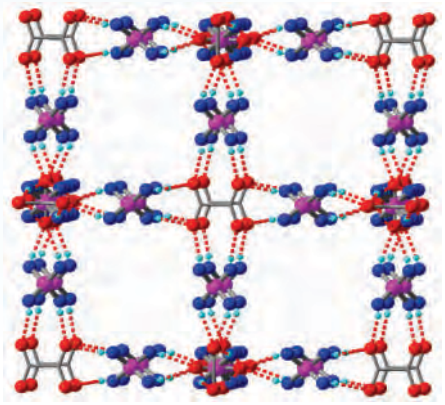




It has also been shown that N-Confused dipyrrin does not show reactivity similar to that of dipyrrins with metal salts. Instead, it undergoes intermolecular cyclomerization, leading to the synthesis of the first examples for expanded norroles. They have multiple C-N bonds along the conjugated pathway of the

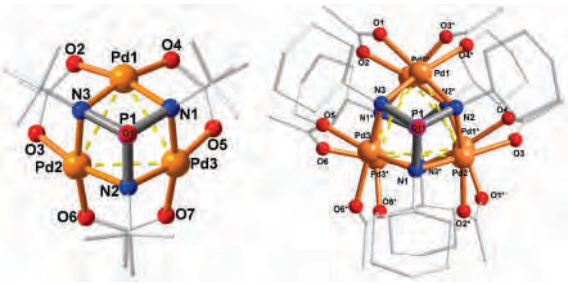
macrocyclic framework. Their synthesis is simple and can be catalyzed by a variety of metal ions. The considerable upfield and downfield chemical shift values signify π delocalization and anti-aromaticity. This macrocycle represents the first example of a 32π octaphyrin with a non-twisted conformation. These macrocycles also demonstrate the possibility of accommodating more than two neo-confused pyrrole moieties and represent a new class of stable anti-aromatic expanded porphyrinoids with unusual π conjugation.

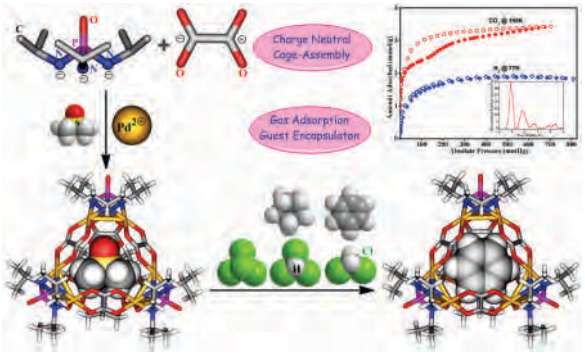
Main group ligands: Multi-Nuclear Cages, Clusters, Functional Materials



The current research focus of **R Boomishankar's** group is on the development of molecular systems derived from the elements of group 13, 14 and 15 and their applications in materials science and catalysis. His group has shown that organoamino phosphonium cations $[P(NHR)_4]^+$ can be used as novel synthons for building designer supramolecular structures aided by hydrogen bonding interactions in presence of various counter anions such as chloride, carboxylate and polyoxometallate ions.

One of the active areas of his research is the facile generation of imido analogues of main-group oxo anions and employing them as ligands in transition metal chemistry. Thus, his group has demonstrated that the imido anions corresponding to $H_2PO_4^-$, HPO_4^{2-} and PO_4^{3-} ions can be obtained by using salts of certain soft transition metal ions such as Ag(I), Pd(II), Cu(I) etc. in reaction with amino P(V) ligands in polar solvents at ambient conditions. It is to be noted that these anions were initially known when amido-P(V) ligands were treated with highly basic organometallic reagents and with limited stability in aprotic non-polar solvents. Reactivity studies on the tris(amido)phosphate ligands of the type $(RNH)_3PO$, with various salts of Pd(II) in methanol have revealed the exclusive generation of the fully deprotonated imido P(V) species analogous to the PO_4^{3-} ion as their tri- or haxanuclear Pd(II) complexes. In addition, the catalytic activity of these Pd(II) complexes in the Mizoroki–Heck (M–H) type coupling reaction of phenylboronic acid with alkenes has been established. Similarly, the imido anions analogous to $H_2PO_4^-$ and HPO_4^{2-} ions can be generated using certain reactive Ag(I) salts from the P(V) moieties having fairly acidic N-*H* groups.

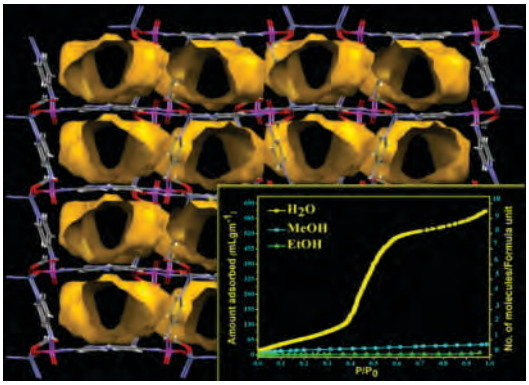




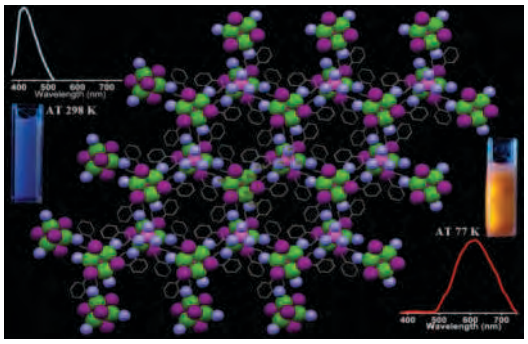
Many of these multi-nuclear Pd(II) complexes possess labile residual OAc groups attached to the Pd(II) atoms and thus are able to undergo further reactions leading to large metalla-supramolecular cages where the tris(imido)phosphate trianion act as a novel cis-blocking agent for a planar Pd_3 building block. The role of this cis-blocking group is to provide stability for the Pd(II) ions and prevent polymerization of these cluster cages. The method utilized for these cages is very unique and aids in the exclusive generation of large charge neutral discrete cages. Furthermore, the tetrahedral cage assembly exhibits remarkable stability and selective gas adsorption and guest solvent encapsulation properties.

The utility of pyridylamino functionalized P(V) compounds such as phosphonium chlorides, phosphine imines and phosphine oxides which offer peripheral binding sites in addition to the imino and oxo sites has been demonstrated

for obtaining larger arrays of metal ions. In a related project, interesting examples of Zn(II)- and Cu(II)-coordination polymers were synthesized for an insitu generated bis(amido)phosphate ligand. Vapour adsorption measurements on these polymers reveal a preferential water uptake in their pores over aliphatic alcohols, promising their application in the purification of Bioethanol.

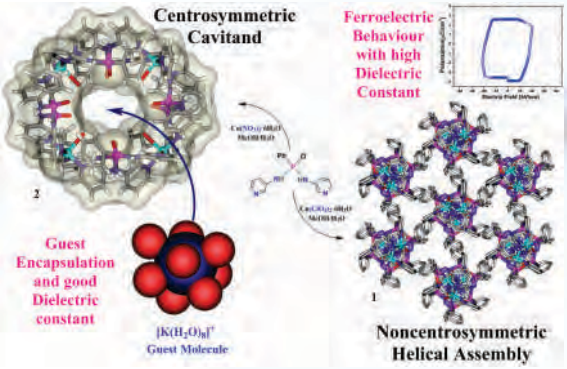


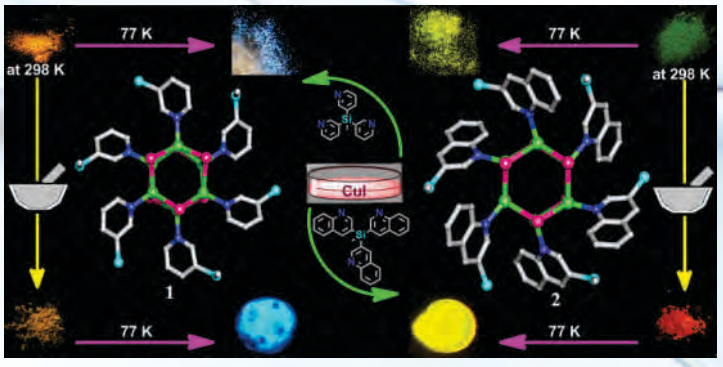
Employing a tripodal aminopyridyl/aminoquinolyl functionalized thiophosphoramide ligands, preparation of C_3-symmetric cationic Rugby-ball shaped $\{[Cu_6I_4]^{2+}\}_n/[Cu_6I_5]^{2+}$ cluster metal-organic frameworks (MOFs) has been achieved. Studies on the photo-physical behavior of these two MOFs indicate their thermochromic luminescent behaviour.



Recently **Boomishankar's** group has discovered that by employing a flexible less symmetric phosphoric diamide ligand featuring neutral pyridyl N-donor sites (L), anion dependant structural assemblies of composition $\{[CuL_2]_n[A]_{2n}\}$ (**1**: n = , A = (ClO_4^-) and **2**: n=4, A = (NO_3^-)) can be obtained. While the compound **1** displays a non-centrosymmetric 1D-helical chain structure, the compounds **2** was obtained as centrosymmetric discrete assembly. Permittivity and ferroelectric studies have shown that counter anions such as perchlorate or nitrate ions can not only control the structural architectures but also can alter the physical properties associated with them. In addition, the hydrophilic central cavity in **2** selectively encapsulates a hydrated potassium cation and excludes other cations such as Na^+ or Cs^+ ion .

His group is also working on ligand scaffolds derived from peripherally functionalized silane and siloxane backbones. Recently, two iso-structural MOF materials **1**, $\{[MeSi(^3Py)_3]_6(Cu_6I_6)\}_n$ and **2**, $\{[MeSi(^3Qy)_3]_6(Cu_6I_6)\}_n$ featuring Cu_6I_6 clusters have been synthesized from tridentate arylsilane ligands. These isostructural MOFs were shown to exhibit thermochromic and mechanochromic luminescence umpolung upon changing the sample temperature and mechanical grinding, respectively. This is primarily due to the variations in their cuprophilic interactions as **1** displays shorter Cu…Cu distances (2.745(1) Å) in comparison with those present in **2** (3.148(0) Å).



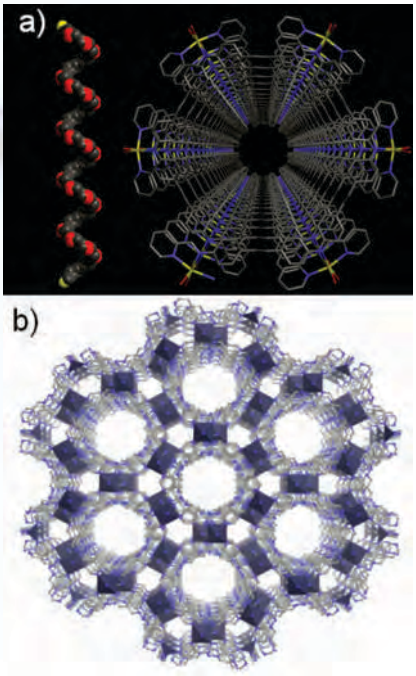


Apart from these, they have also been working on other silane and cyclic siloxane based ligands containing peripheral functionalities. Such ligands have led to the isolation of interesting designer architectures in cage and polymeric structures. Application of some of these cage molecules in host-guest chemistry and reactions within its confined space are in the process.

Metal Organic Frameworks

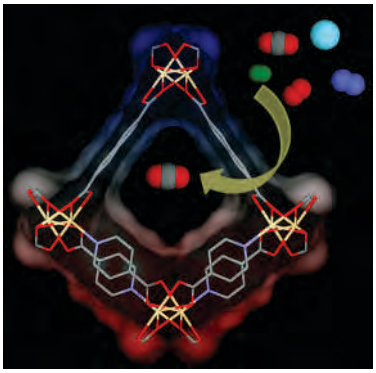
The principal research focus of **Sujit Ghosh's** research lies in the development of functional porous materials based on coordination polymers, suitable for applications in chemical industries, energy & environmental issues. Self assembly of predesigned organic building units (linkers) and metal ions/clusters involving appropriate coordination affinity allows the formation of the desired multidimensional networked structures known as Metal-Organic Frameworks (MOFs) or Porous Coordination Polymers (PCPs). Over the last decade, these organic-inorganic hybrid materials have particularly proved their excellent credibility for proficient application in the fields of gas storage and separation, catalysis, ion recognition, chemical separation, ionic conductivity, sensing etc.

The group seeks to correlate the designed structural features with intriguing physical properties and to design new synthetic methods to prepare functional materials and consequently tuning their properties from the standpoint of structural design.

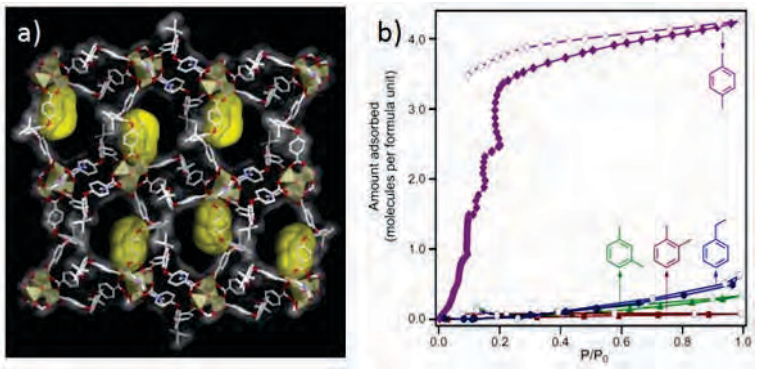


Crystalline porous Metal-organic frameworks (MOFs)

Carbon capture and storage (CCS) technology is seeking great attention in the recent years owing to the pressing issue of greenhouse gas emissions, especially CO_2, which is directly linked to global warming & climatic changes. In particular, MOFs are seeking overwhelming attention due to high surface areas. Some of our new materials presented excellent CO_2 selectivity. The group has reported moisture stable 2,6-napthalene dicarboxylate and isonicotinic acid based Cd(II) porous MOF with pore size ~8 Å for selective CO_2 capture over N_2, H_2, Ar, O_2,CH_4 gases.



Selective capture of CO_2 by porous MOF over N_2, H_2, Ar, O_2, CH_4 gases.

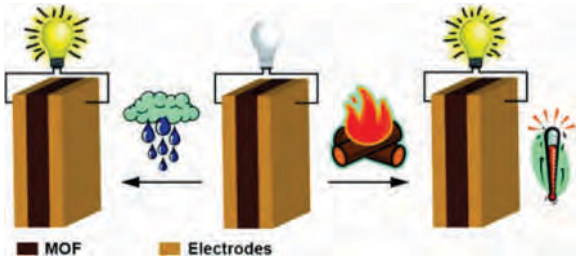


Selective adsorption para-xylene over its congener isomers by a Zn(II) based flexible MOF

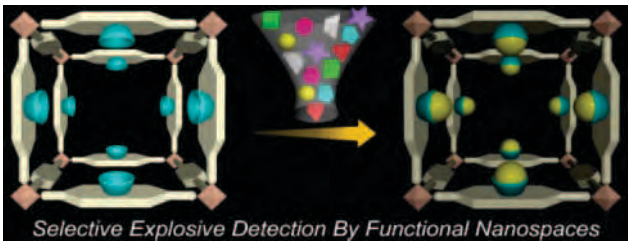
Chemical separation has immense importance in industrial applications. Separation of industrially vital monomers like benzene, *p*-xylene and styrene from the congener product streams is being investigated through construction of novel MOF materials and by appropriate exploitation of framework flexibility, open metal sites, lewis acidity etc. Recently, our group came up with the demonstration of an unprecedented selective adsorption phenomenon of para-xylene over its congener isomers by a new Zn(II) and carboxylate based flexible MOF.

Fuel cell as a clean energy source is emerging as an attractive option to produce energy in higher efficiencies without environmental pollution. MOFs offer a feasible alternative to overcome the intrinsic constraints of the currently used

Nafion membranes. The group has designed oxalate based Zn(II) MOF with hydrogen bonded dimethyl ammonium cations and sulphate anions for both anhydrous and humidified conditions. The humid condition conductivity is reported to be 4.2×10^{-2} S cm^{-1} which is amongst highest value known for MOF and is the first report of MOF which shows proton conductivity in both humid and anhydrous condition.



Schematic representation of humid and anhydrous proton conduction by MOF based solid electrolyte



Porous MOF decorated with Lewis basic sites (pyridyl /amine) for aqueous phase selective TNP detection.

MOFs as chemical sensor to induce luminescence as the signal transduction mechanism has been employed for addressing major security concerns like explosive detection. This has been achieved by appending Lewis basic pyridyl or amine functionality as recognition site into the porous channels of fluorescent Zr (IV) MOFs. First time the aqueous phase selective detection of 2,4,6-trinitrophenol (TNP) in presence of competing nitro analytes is demonstrated using MOF as probe. The detection limit for TNP was found to be 0.6 ppm.

The exploration of diverse functional aspects for different types of porous materials, mostly, MOFs and covalent-organic frameworks (COF) towards new-generation advanced porous materials for potential applications in energy and environmental needs are in progress.

Advance Porous Materials: MOFs & COFs

Ramanathan Vaidhyanathan's research is focused on the synthesis of porous framework materials including Metal Organic Frameworks, Covalent Organic Framework and ceramic based systems. The project aims to develop methods that avoid 'interpenetration' associated with MOFs. The crystallographic analyses of these MOFs show that even with closely related iso-compositional MOF structures, the openness or porosity could be varied by introducing asymmetry into the overall topology, that could be effected by synthetic control.

Another important focus of the group is towards tuning the CO_2 capture/separation capabilities of microporous MOFs. Synthetic strategies are used to control the capacity and selectivity for CO_2 in a Zinc amino triazolate family of MOFs. Several iso-compositional MOFs have been made and all with similar layered-pillared topology. In all cases, the Zn-aminotriazolate layers are pillared by oxalate units. However, the subtle differences in the corrugations associated with the layers create differences in the topology which can be monitored by the dihedral angles it makes with the pillars. It is possible to control this tilt or dihedral angle

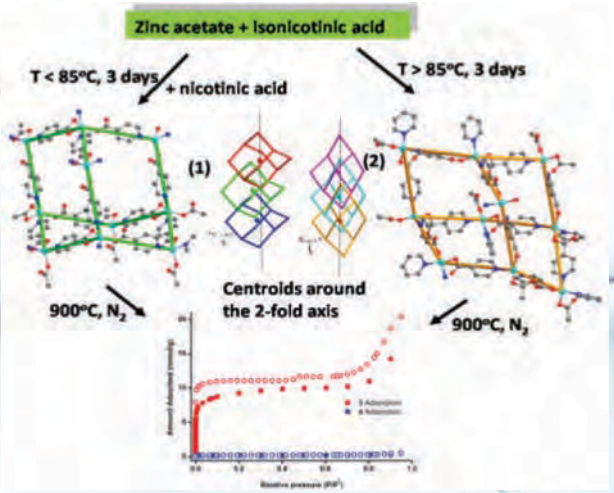


Figure shows the diamondoid structure of a Zn(isonicotinate)2 MOF. Note how the disposition of the diamondoid about the 2-fold axis is different in the two different diamondoid nets that have been shown.

by synthetic methods. Now, this has a direct consequence on the pore size and shapes in the 3-D structure. It also affects the exposure of specific functional groups on to the free spaces within the nanopores. Based on these insights a suitable preparation method and condition that has most porous ZnAtzOx framework which reaches nearly the theoretical capacity estimated from its single crystal structure. been identified.

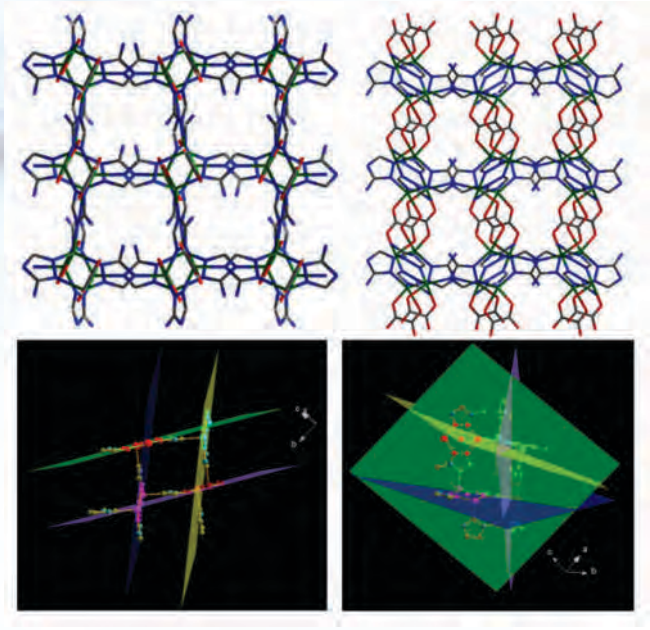


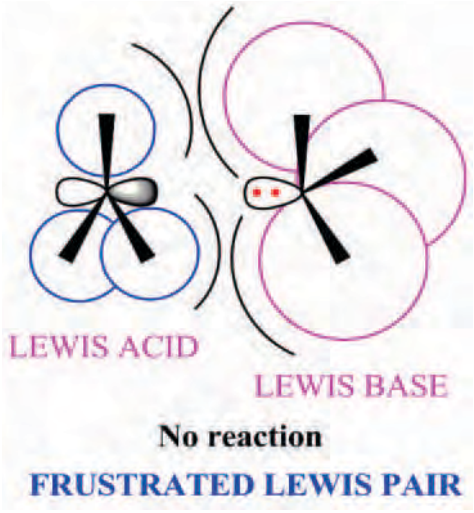
Figure shows two different 3D MOFs formed using Zn-aminotriazolate-oxalate units with different topologies and a crystallographic analysis gives insight into how the layer displacements correlate to openness.

Main Group Cations and Catalysis

The controversy over "how free the trivalent silicon cation is" has led to emphasis on their spectroscopic and crystallographic characterization and to understand the role of *s* or *p* Lewis basic molecules culminating in the discovery of innocent (*non-coordinating*) anions.

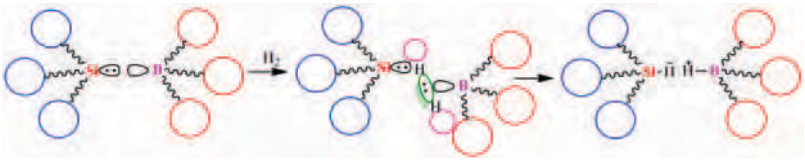
Silylium ions are extremely strong Lewis acids due to the electron sextet at the silicon atom and these electron deficient compounds are promising reagents in catalysis.

The major drawback of model (designed) catalysts is inadequacy of turnover numbers due to the instability of the counter-anion. To overcome the limitations, and design powerful catalysts, **Shabana Khan**'s group is working on synthesis of silylium ion using $[B_{12}Cl_{12}]^{2-}$ (as non-coordinating anion).



Her group is also involved in the development of Si-based frustrated Lewis pair which can be utilized further to activate small molecules.

The FLPs have a Lewis acid and a Lewis base functional group, which cannot make a dative bond with each other because of the bulky substituents attached. The resulting reactive center in the molecule pair can easily activate small molecules, for example the dihydrogen.



In some cases this activation is reversible which is very important because the catalysts should be able to release the hydrogen. Thus, the excessive stability of the products is undesirable. Reversible activation of gases offers new pathway for gas storage and catalytic reduction.

Main Group Chemistry: Catalysis and Materials Applications

The last two decades witnessed the exuberant growth of the chemistry of heavier main-group elements. Arguably, the heavier main-group elements have fundamentally different electronic properties from their lighter congeners. With the discoveries of heavier main-group compounds in their low-valencies, the common perceptions such as their colourless nature, large HOMO-LUMO gaps, inertness towards bond activations, etc. have been invalidated. Worth mentioning features of such low-valent compounds are the following: (1) multiple bonds between them; (2) low-valent species with open coordination sites; (3) radical species etc. All these species have in common, frontier orbitals with small energy separations, which in turn resembles the well-explored transition metal complexes.

Moumita Majumdar's research focus is to expand the chemical functionalities of low-valent compounds spanning the Groups 13-15 of the periodic table. Such functionalities will be translated to provide solutions to technological problems, catalytic applications and also replace expensive precious-metals in small molecule activations, catalysis etc. The programme involves two broad research targets:

1. Development of Main-Group Polymers featuring Homo/Hetero-nuclear Double Bonds: In carbon chemistry, the HOMO-LUMO gap is lowered by conjugation of the double bonds in the polymer chain, which is the underlying principle for their applications in electronic and photonic devices. The aim is to synthesize poly(phenylenevinylene) (PPV) analogues involving homo- or hetero-nuclear bonds in the polymer backbone that will conceptually mimic inorganic semiconductors such as gallium phosphide or indium arsenide.

2. Applications of Multiply Bonded Transition Metal-Silicon Based Compounds: The group will explore the stability of newly synthesized multiply bonded transition metal-silicon compounds and their potential applications. The transition metal and low-valent silicon working in tandem, will be utilized in the fields of catalysis, coordination polymers, conducting materials etc.

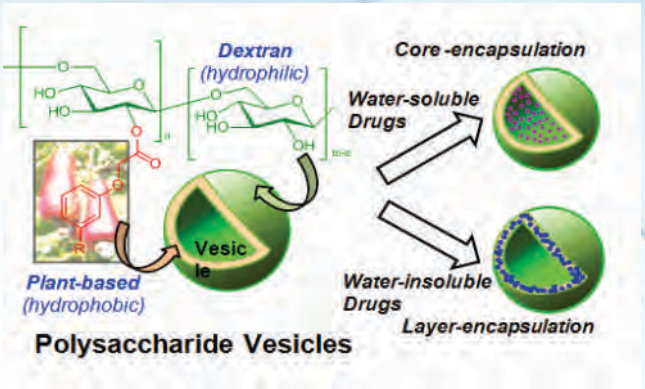
Recent literature have pointed to viable transition-metal surrogates by steering their frontier orbitals and energy separations. The long-term target of the group is to stabilize metal-free main-group compounds in order to primarily utilize them for small molecule activations and eventually turn them into prospective catalysts.

C. Materials, Nanoscience, Polymers and Surface Science

Polymer Science

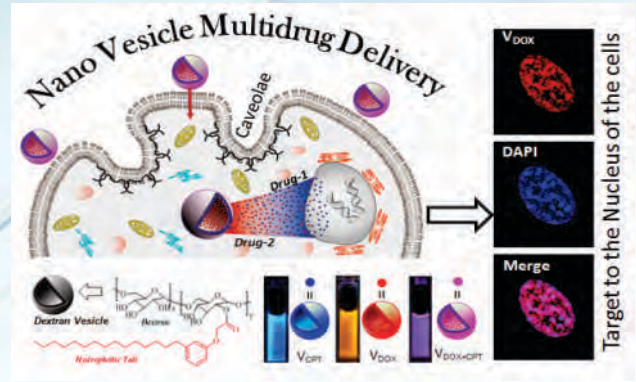
Jayakannan's research group has been working in the area of polymer science. Biodegradable and biocompatible polymer scaffolds for delivering anticancer drug molecules, new solvent free and eco-friendly melt condensation processes for amino acid based polymers, and supramolecular assemblies of π-conjugated polymers for opto-electronics are developed in his group.

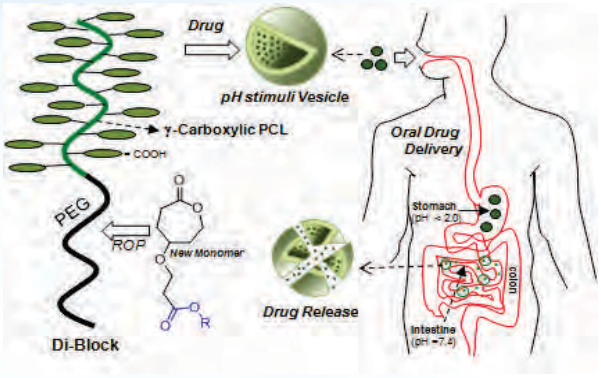
Polymers for Drug Delivery: Polymer based nano-assemblies are emerging as an important tools for the administration of medicines or genes in cancer treatment. His research group has developed the following polymer system for the drug delivery applications: (a) Responsive Polysaccharide Vesicular nano-scaffolds, (b) Poly(caprolactone) functional Block copolymers and (c) Thermo-responsive A-B Diblocks.



His research group has developed unique dextran vesicles that were capable of protecting the plasma sensitive CPT lactone pharmacophore against the hydrolysis ten times

better than the CPT alone in PBS. Recently, the approach has extended to multiple drug loading and sequential drug delivering polysaccharide nano-vesicle for administering anticancer drugs DOX (topoisomerases II inhibitor) and CPT (topoisomerases I inhibitor) to achieve synergistic killing of cancer cells.

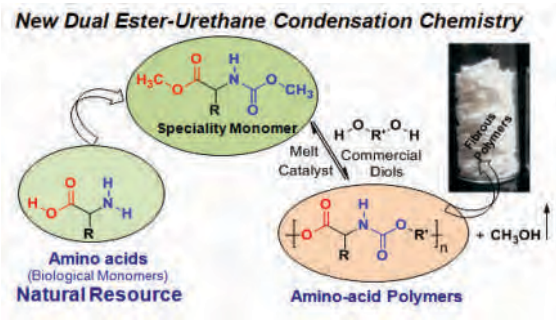




His research group has designed new pH responsive carboxylic functionalized polycaprolactone (PCL) block copolymers. These carboxylic substituted PCL block copolymers were self-assembled as pH responsive polymer vesicles in water for loading and delivering of drugs. These new vesicles were successfully demonstrated as delivery vehicles for both hydrophilic molecules (like rhodamine B, Rh-B) and hydrophobic drugs (Ibuprofen, IBU and camptothecin, CPT) under simulated GI tract.

These pH responsive PCL vesicles were stable in strong acidic conditions (pH < 2.0, stomach) and ruptures to release the loaded cargoes under neutral or basic pH (7.0 = pH) similar to that of small intestine.

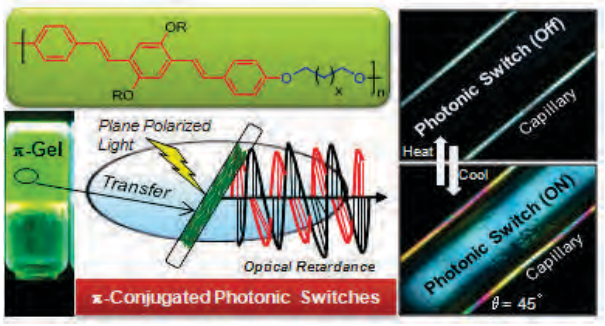
Eco-friendly Synthetic Approaches for Polymers: Discovery of new green chemistry routes to replace existing hazardous ones is an important area of research for cleaner and environmental friendly industrial developments. His group has demonstrated *a novel melt transurethane* process for a commercially important class of polymers –polyurethanes. The present synthetic strategy is very good in producing urethanes and polyurethanes under solvent free conditions and very efficient for producing high molecular weight polymers compared to that of isocyanate routes.



Recently, a new dual ester-urethane melt condensation methodology for biological monomers-amino acids was developed to synthesize new classes of thermoplastic polymers under eco-friendly and solvent free polymerization approach. Naturally abundant L-amino acids were converted into dual functional ester-urethane monomers by tailor made synthetic approach. The current investigation opens up new platform of research activates for making thermally stable and renewable engineering thermoplastics from natural resource -amino acids.

Polymers for Electronics: Jayakannan's research group has developed new molecular designs in the π-conjugated molecules which could only self-organize through weak non-covalent forces. New series of bulky oligophenylenevinylenes (OPVs) have fixed aromatic π-core with variable chain in the longitudinal position were

designed. These molecules were self-organized into three dimensional supra-structures via chlolestric liquid crystalline (LC) mesophases.



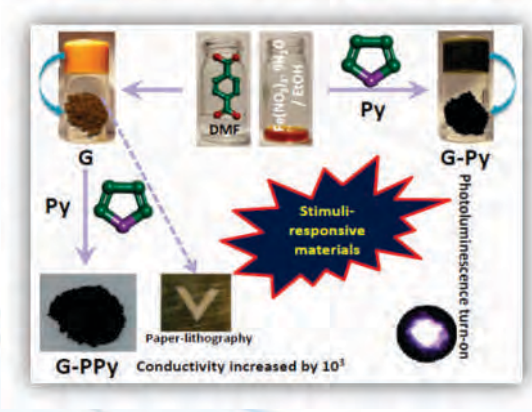
Recently, his group has demonstrated one of the first examples of π-conjugated photonic switches (or photonic wave plates) based on the tailor made π-conjugated polymer anisotropic organogel. New semi-crystalline segmented π-conjugated polymers are designed with rigid aromatic OPV π-core and flexible alkyl chain along the polymer backbone.

These semi-crystalline polymers produce organogel having nano-fibrous morphology. The polymer organogel is aligned in a narrow glass capillary and this anisotropic gel device is demonstrated as photonic switches. The glass capillary device behaves as typical λ/4 photonic wave plates upon the illumination of the plane polarized light. Thermo-reversibility of the polymer organogel (also its xerogel) was exploited to construct thermo-responsive photonic switches for the temperature window starting from 25 to 160°C.

Surface Science and Materials Chemistry

Metal-Organic Gels and Hybrids

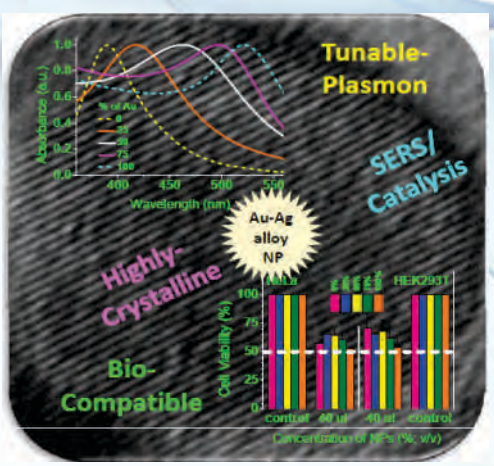
Polymeric coordination of organic ligand to metal ion leads to the formation metal-organic frameworks and metal-organic gels. The properties like visco-elasticity and stimuli-responsive behavior are added advantages in metal-organic gels.



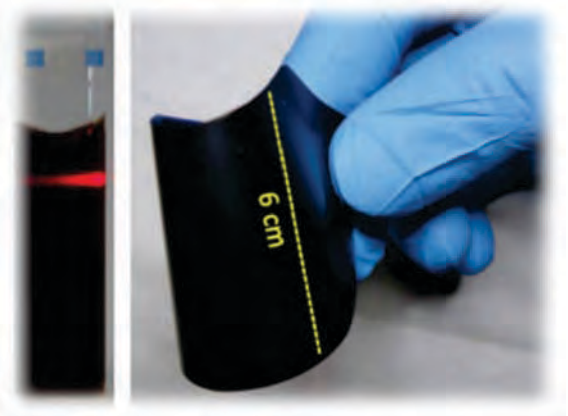
Fe-BTC/TPA (benzene tricarboxylic acid/terephthalic acid) gels has been utilized to incorporate in situ (without the use of extraneous oxidant) conducting polymers polypyrrole and polythiophene which resulted in the generation of conductive composite materials similar to earlier studied *polymer bronzes*. Also, we have used pyrrole, bithiophene and aniline as the co-ingredients of the redox-active Fe-TPA gel to turn-on the photo-luminescence which is otherwise non-luminescent. Ongoing activities in this direction include diode characteristics and photovoltaics.

Plasmonic Nanoparticles

Alloy NPs is a very active field of multidisciplinary research with promising applications in photonics, plasmonics, sensing, medical diagnostics and catalysis. Wet-chemistry has been playing a pivotal role in producing stable Au-Ag alloy NPs with controllable structure-property relationship via standard co-reduction of $HAuCl_4$ and $AgNO_3$. A detrimental factor in co-reduction persisting over a decade period is the co-precipitation of AgCl which adversely affects the composition and various properties; thereby always pushed the limit of standard co-reduction below the solubility product of AgCl! Another alarming concern is the surface-enrichment of Ag in the Au-Ag alloy NPs which has been majorly overlooked on the basis of the similar lattice constants of Au and Ag.



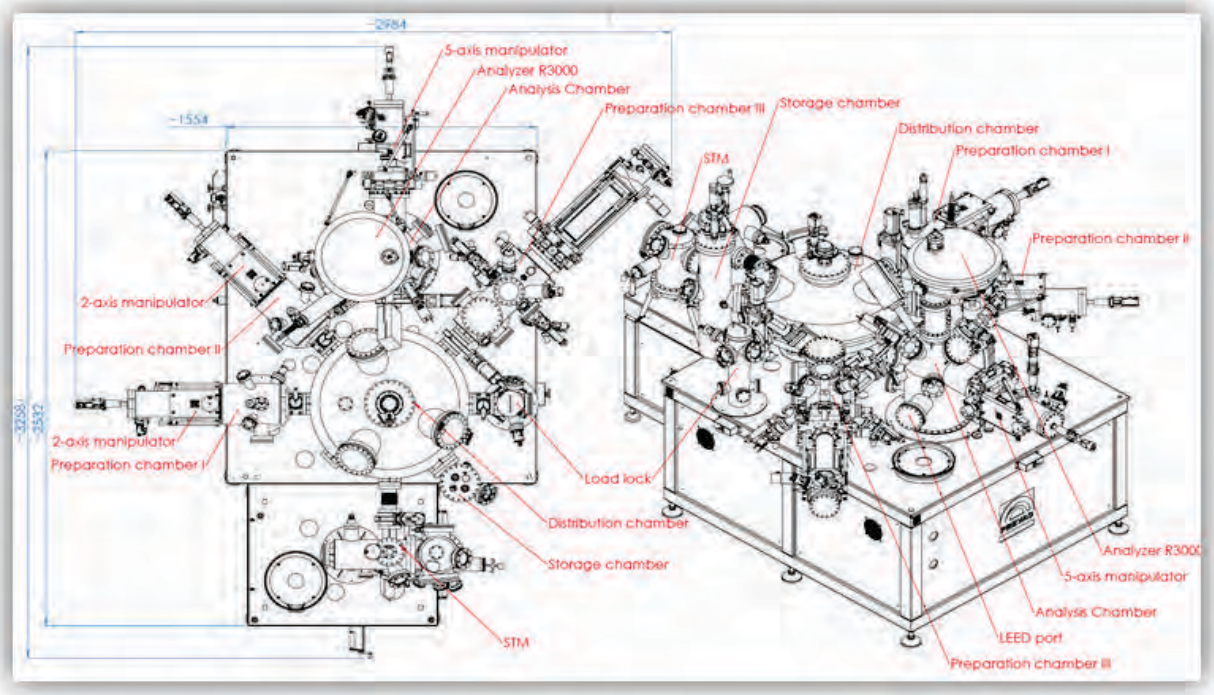
Nirmalya Ballav's group is working to address the concept of 'true-alloying' of Au and Ag in NPs by exploring the power of wet-chemistry as well as combining various complementary measurements. This work is expected to stimulate future investigations in the development of *multifunctional alloy NPs* with high-performance capability.



Chemically Converted Graphene

Graphite oxide (GO) is one of the main precursors to generate graphene-based materials, which are highly-promising for various technological applications. Currently the wet-chemical route to produce so called *chemically converted graphene* (CCG) sheets with thickness in the range of few mm and length in the range of few cms is being explored. Specifically, the group is interested in the thermal and electronic properties of flexible CCG thin-films.

Establishment of Surface Science lab: At the forefront of scientific and technological evolution lies controlled experimentation and engineering with individual molecules, atoms, and quantum states. This is where current *Surface Science* – the art of keeping surfaces atomically clean and chemically well-defined; and *Nanoscale Science* – the art of controllably fabricating, manipulating and experimenting with small objects meet. Progress at the frontier of Surface Science research critically depends on highly-specialized equipments which combines spectroscopy (XPS/UPS) and microscopy (STM) techniques. At IISER Pune a dedicated facility is planned which enables the Institute in performing cutting-edge research in this highly-visible and dynamic field towards fundamental understanding and future technological applications. This facility will be a very important and useful addition to the existing facilities at IISER Pune.

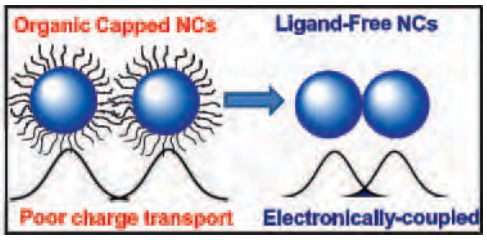


Surface Science Laboratory @ IISER Pune

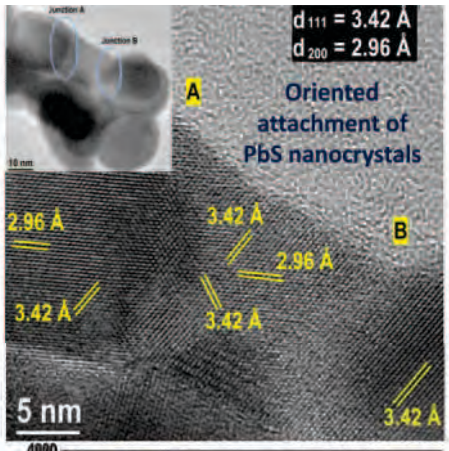
Colloidal Semiconductor Nanocrystals

The main research focus of **Angshuman Nag's** group is on developing functional inorganic materials using solution processed semiconductor nanocrystal modules. The work can be divided in to three major sections (i) material design mainly using colloidal organic-free nanocrystals, (ii) spectroscopic studies using luminescence and XAFS, and (iii) magneto- and opto- electronic applications forming flexible transparent conductor, solar cell and carrier mediated magnetic coupling.

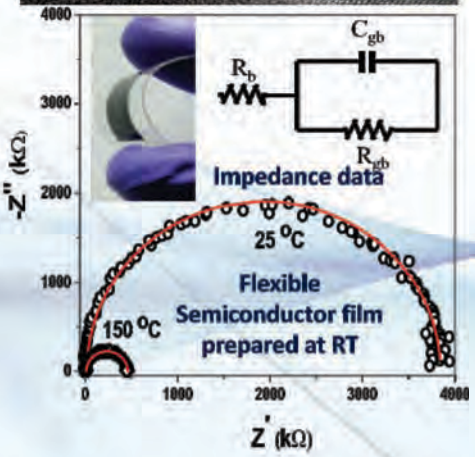
Electronically Coupled All-Inorganic Nanocrystals



Integration of nanocrystals in electronic and optoelectronic devices like photovoltaics, light-emitting-diodes (LEDs), photodetectors and printable electronics depends on the electronic property of the nanocrystal film, and thus on the interconnect between adjacent nanocrystals. However, colloidal nanocrystals are generally capped with an insulating organic layer. Consequently, the benefits of quantum confinement effect and solution processibility cannot be utilized because of inefficient injection or extraction of charge carriers. Nag's group is interested in designing organic-free semiconductor nanocrystals for various optoelectronic applications. They have developed a novel synthesis protocol for preparing colloidal ligand-free metal chalcogenide nanocrystals (CdS, ZnS, Mn-doped $Zn_{1-x}Cd_xS$, CdSe, ZnSe, PbS, PbSe, and $AgInS_2$). These ligand-free nanocrystals exhibit signature of electronic coupling in a nanocrystal film, and have been employed to prepare non-toxic and less explored $AgInS_2$ quantum dot sensitized solar cell. Ligand-free Sn doped In_2O_3 and $AgInS_2$-Ag_2S heterodimers are being investigated to achieve solution processed flexible transparent conducting oxides and in-built p-n junction for photovoltaic applications, respectively.



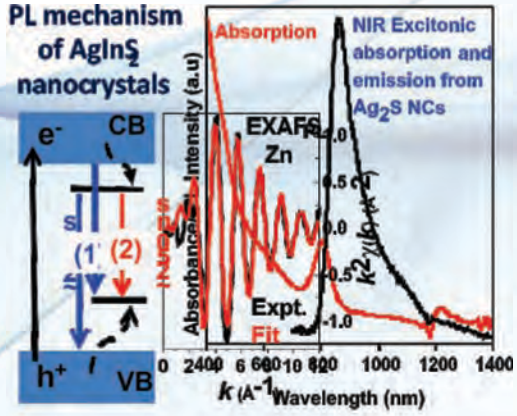
Sintering of solution processed semiconductor nanocrystal has been recently recognized as an easy and cost-effective method to grow semiconductor thin films. Typically, the nanocrystals need to be sintered at >350 °C. However, such high temperatures are not suitable for flexible polymer substrate. Nag's group developed a novel method to sinter ligand-free PbS and PbSe nanocrystals at room temperature employing oriented attachment of nanocrystals.

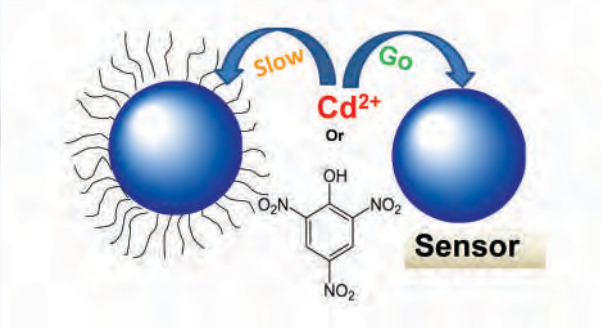


Luminescent Nanocrystals

I-III-VI_2 semiconductor (for example, $AgInS_2$ and $CuInS_2$) nanocrystals exhibit a new kind of luminescence different from both excitonic emission and dopant-related emission. Nag's group elucidated the luminescence mechanism for colloidal $AgInS_2$ nanocrystals. There are two radiative pathways, one involves delocalized states like valence and conduction band, and the other path way involves two localized donor and acceptor defect states.

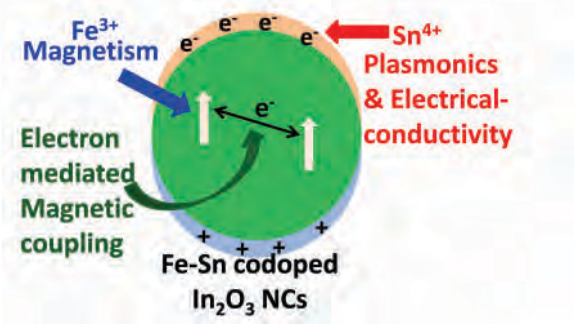
Ag_2S nanocrystals have been studied in recent times because of its near infrared luminescence. Typically, broad absorption and luminescence are observed from Ag_2S nanocrystals. Nag's group developed Ag_2S nanocrystals exhibiting narrow excitonic absorption and emission.





In another interesting approach, organic-free luminescent nanocrystals have been developed for chemical sensing simply utilizing the fact that the analyte can interact easily with the bare nanocrystal surface.

Doped Semiconductor Oxides

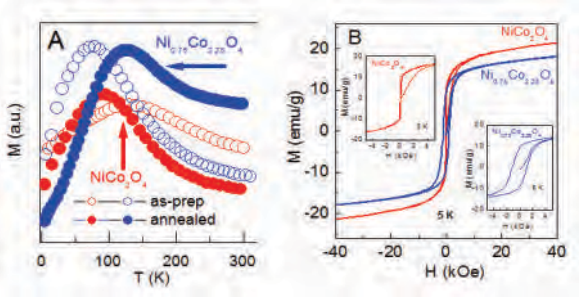


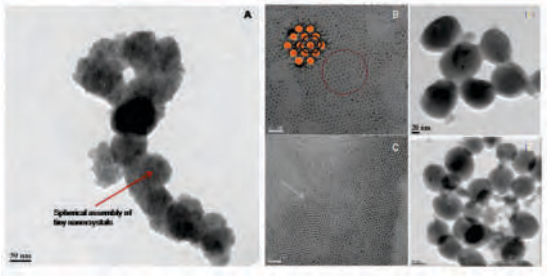
Nag's group is developing a unique category of material exhibiting the above mentioned three properties simultenously, via doping a magnetic ion in a transparent conducting oxide nanocrystal. For example, in Fe-Sn codoped In_2O_3 nanocrystals, localized surface plasmon resonance band is observed in near to mid infrared region along with room temperature ferromagnetism and electrical conductivity >1 S/cm. More importantly, the electron mediated magnetic coupling can lead to spin based applications.

Multifunctional Magnetic Nanoparticles

The main research focus of **Seema Verma's** laboratory is to develop novel synthetic routes to synthesize highly monodispersed multifunctional magnetic nanocrystals using suitable surfactants that are dispersible both in water. The group is also focusing on designing multifunctional magnetic-plasmonic hybrid nanostructures by utilizing novel synthetic routes. Emphasis is given to obtain mesoporous magnetic-plasmonic hybrid materials, suitable for biomedical applications and in active plasmonic devices. Further work is going on to obtain the nanohybrid structures suitable for SERS applications. The group has reported a strategy to obtain a stable thin film of magnetic nanocrystals at the air/water interface utilizing Langmuir-Blodgett (LB) method. This strategy can be extended to any similar systems.

Recently, the group has reported a detailed examination of the effect of induced off-stoichiometry on structural, thermal and magnetic properties of nickel cobaltite, $NiCo_2O_4$ nanoparticles which is a promising transparent conducting oxide material. It is seen that the excess cobalt ions stabilize the nickel cobaltite structure even up to the temperature of 773 K and has interesting consequences on the magnetic structure and properties. Enhanced thermal

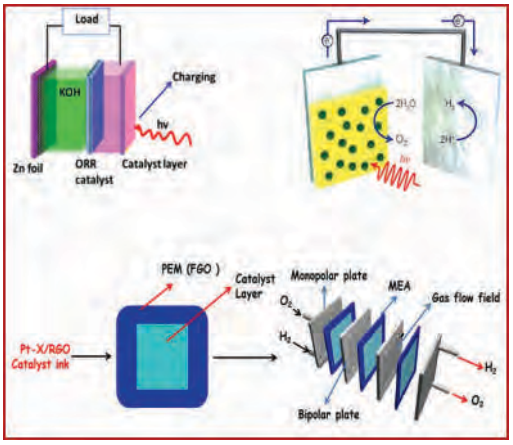




stability, improved structural and magnetic properties of the off-stoichiometric sample is evident from the magnetic and neutron diffraction studies.

A comparison of zero-field cooled (ZFC) magnetization of off-stoichiometric ($Ni_{0.75}Co_{2.25}O_4$) and stoichiometric ($NiCo_2O_4$) nanoparticles show stronger exchange interaction value for annealed off-stoichiometric samples. This observation was well supported by the field dependent magnetization measured at 7K. Off-stoichiometry in nanosystems may thus offer a novel route to new materials with interesting properties.

Energy and Electrochemistry

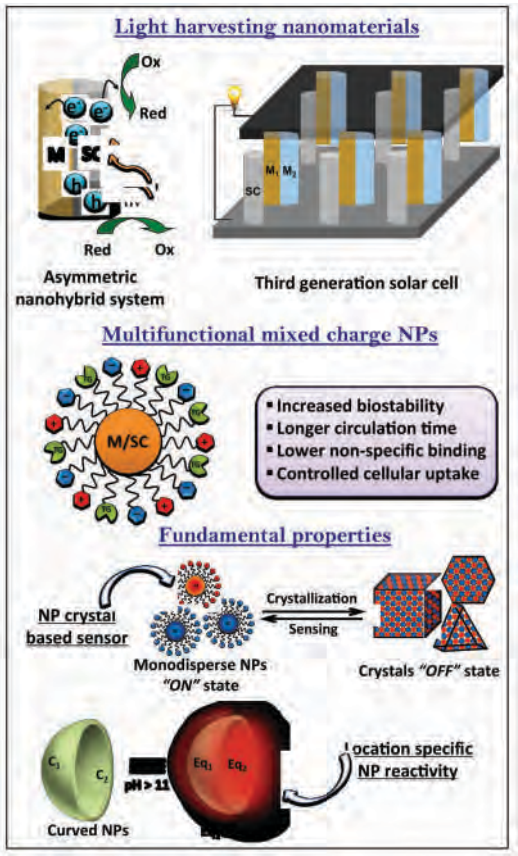


The development of novel energy generation and storage techniques presents chemistry with its possibly most important challenge of the 21st century. The rechargeable lithium-ion battery has revolutionised portable electronics, however Li-ion batteries, with $LiCoO_2$ and Li transition metal oxides as the Li active materials, used widely today face serious problems relating to safety and resource costs.

The main research focus of **Musthafa's** energy laboratory is understanding the complex phenomena at the electrode/electrolyte interface by a range of electrochemical, microscopic and spectroscopic techniques and extending the fundamental understanding gain at the molecular level to design cost effective, economical and environmentally friendly energy storage and conversion devices. Further, his group has interest in building novel interfaces for selective sensors, water splitting, photoelectrochemical production of fuels, water remediation etc.

Towards this direction the group has interests to explore: (i) the photo charging batteries to decrease the higher charging voltages and longer charging time and (ii) the self-discharge encountered in typical energy storage devices, developing novel proton exchange membranes for PEM fuel cells towards new energy storage and conversion strategies.

Nanomaterials for Light Harvesting and Biotargeting Studies



Research in **Pramod Pillai's** laboratory is focused on the design and synthesis of hybrid nanomaterials formed by the integration of two or more materials at the molecular or nanometer length scale which may exhibit fundamentally new properties and phenomena. Nanomaterials based on organic-inorganic, metal-metal and metal-semiconductor nanomaterials will be developed to address two global concerns: (1) energy and (2) therapeutics.

The goal of **Pillai's** group is to improve the stability of the charge separated species in light harvesting materials to improve their overall efficiency. Efforts are to develop heterostructures based on metal (M) and semiconductor (SC) nanomaterials for studying the effect of geometries, compositions and configurations on the stability of photogenerated electron-hole pairs. The inclusion of

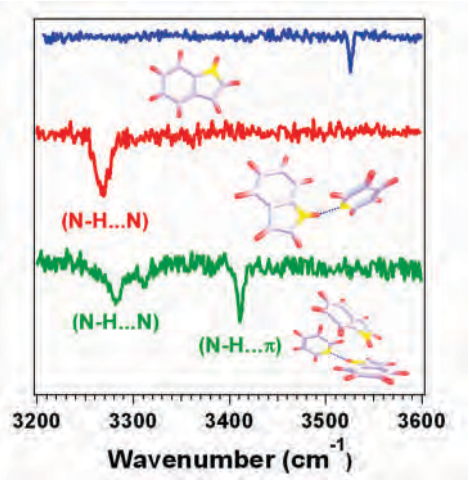
metal nanostructures, as one of the components, is expected to enhance the overall efficiency of the photovoltaic device due to its (i) electron storage/transport capability and (ii) light concentration property through a strong near-field enhancement by the surface plasmon effect.

Another area of focus is on providing insights into the basic question in nanomedicine: how to improve the biostability and specific targeting of nanomaterials in therapeutics. The surface chemistry (charge, functionality, ligand arrangement, hydrophobicity and hydrophilicity) plays a crucial role and improvement for tuning simultaneously incorporation of ionizable and biotargeting. These multifunctional NPs are anticipated to exhibit advanced biophysical properties such as improved biostability and circulation time, controlled cellular uptake, reduced non-specific binding etc.

D. Spectroscopy and Dynamics

Gas Phase Laser spectroscopy

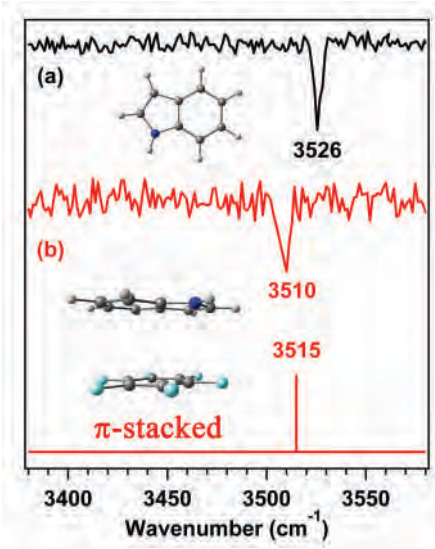
The major research focus of **Aloke Das** and his group is on molecular level understanding of weak non-covalent interactions responsible for the stabilization of specific structures of biomolecules (proteins, DNA etc.) and biological recognition processes. The primary thrust of the research is to unravel the detailed nature and strength of these interactions as well as competition among these non-bonding interactions. In-depth knowledge about these interactions is extremely helpful in designing efficient drugs and functional materials. Mass-selected electronic and vibrational spectroscopy of weakly-bound complexes of the building blocks of biomolecules and materials are studied in the isolated gas phase (supersonic jet) employing UV and IR laser based various spectroscopic techniques combined with quantum chemistry calculations. The spectroscopy experiments are performed in a home-built REMPI (Resonantly Enhanced Multiphoton Ionization) jet-cooled Laser Desorption Time of Flight Mass spectrometer. A glimpse of a few ongoing projects is highlighted here.



Non-covalent interactions: Molecular level understanding

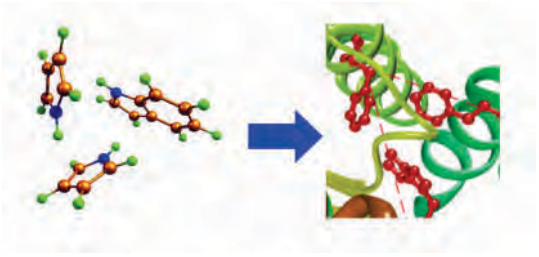
Das's group work on spectroscopic studies of ***"special class of mixed complexes"*** comprising of strong hydrogen bonding and dispersion bound interactions (multiple types of non-covalent interactions) has revealed unique information on the basic structures of biomolecules and materials.

Das and co-workers have studied mixed dimer and trimer of indole and pyridine synthesized in a supersonic jet using Resonant 2-Photon Ionization (R2PI) and IR-UV double resonance spectroscopic techniques. It has been observed that indole...pyridine dimer has a unique V-shaped geometry while $(indole)_2$...pyridine trimer has a cyclic structure. It is intriguing to note that such geometry of the complexes is formed to gain maximum stability through effective use of hydrogen bonding and dispersion interactions. They have shown here how the geometry of molecules and complexes are governed by delicate balance between strong hydrogen bonding and dispersion interaction.



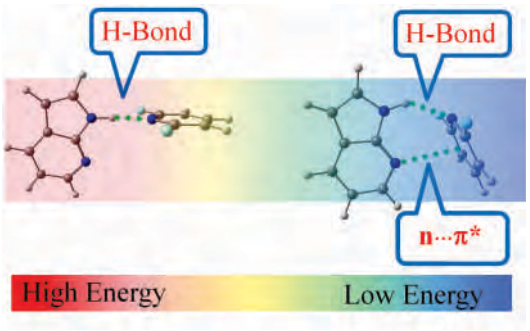
Exclusively π-stacked heterodimer of indole and hexafluorobenzene has been observed in the gas phase by using R2PI and IR-UV double

resonance spectroscopy combined with quantum chemistry calculations. It has been found that the observed π-stacked indole...hexafluorobenzene dimer has a unique structure where the center of the hexafluorobenznene ring is aligned with the center of the shared bond of the indole ring. This work demonstrates that hexafluorobenzene in comparison to benzene is a superior building block for designing very stable material with infinite columnar structure through -stacking interaction and less slip angle between two molecular units.



Aromatic-aromatic interactions are of profound significance in the stabilization of the specific functional structures of proteins as well as protein-protein and protein-ligand interactions. The Das group has studied aromatic trimeric interactions which are very often present in the aromatic side chains of proteins. They have reported here a direct experimental evidence of the observation of a cyclic asymmetric triangular structure of indole···(pyrrole)$_2$ trimer held by three N-H···π hydrogen bonding interactions. The structure observed in the experiment resembles with a trimeric structure of tryptophan and two phenylalanine residues in the crystal structure of a protein called L-ribulose-5-phosphate 4-epimerase (PDB ID: 1JDI).

n →π*interaction: Spectroscopic evidence



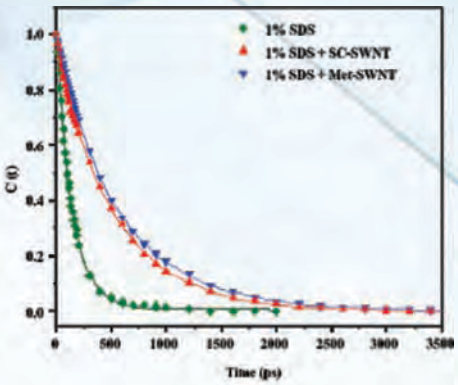
In this work, Das group has studied a subtle competition between a very weak n→π^*_{Ar} and a very strong hydrogen bond (N-H...N) interactions present in the complexes of 7-azaindole with a series of 2,6-substituted fluoropyridines and observed how the weak interaction modulates the overall structural motif of these complexes in the presence of the strong interaction. They have proved the presence of the n→π^*_{Ar} interaction by probing the strength of the hydrogen bond (N-H...N) through measurement of the N-H stretching frequency using IR-UV double resonance spectroscopy.

Future work of Das group includes direct spectroscopic evidence of the n→π^*_{Ar} interaction by probing carbonyl stretching frequency, gas phase study of sequence dependent folding motifs in peptides by using laser desorption jet-cooled study, vibrationally resolved CD (Circular Dichroism) spectroscopy of different conformations of peptides and other chiral molecules in isolated gas phase.

Fluorescence Spectroscopy, Excited State Dynamics and Biophysics

The main research focus of **Partha Hazra's** laboratory is to study the excited state photophysics and dynamics of fluorophores/drugs in molecular containers, various kinds of self-assembled organized structures as well as in biologically tailored systems.

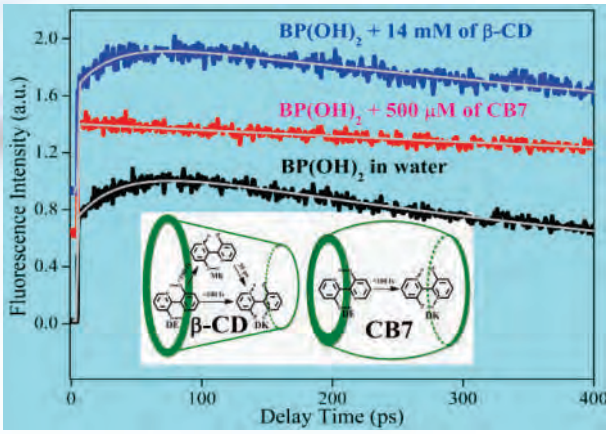
Ultrafast Fluorescence Dynamics



The group has studied the solvation dynamics and rotational relaxation of Coumarin 153 (C-153) in SDS dispersed two different types of single walled carbon nanotubes (SWNTs), namely metallic and semiconducting, using picosecond fluorescence spectroscopy. It has been observed that solvation dynamics of C-153 in SWNTs is severely retarded compared to pure water and SDS micelle.

In another work, urea dynamics inside AOT reverse micelle (RM) has

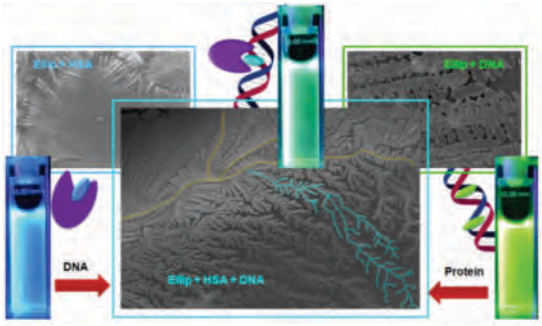
been monitored without intervention of water using time resolved fluorescence techniques from picosecond to nanosecond time regime. It has been observed that urea dynamics inside the reverse micelle is severely retarded compared to water RM due to the formation of highly networked urea cluster inside the RM.



Femtosecond fluorescence upconversion measurements are employed to elucidate the mechanism of ultrafast double proton transfer dynamics of $BP(OH)_2$ inside molecular containers (cucurbit[7]uril (CB7) and β-cyclodextrin (β-CD)). Femtosecond up-converted signal of $BP(OH)_2$ in water consists of growth followed by long decay component (~650 ps). The apperance of growth component (~35 ps) in the up-converted signal indicates the presence of two-step sequential proton transfer process of $BP(OH)_2$ in water. Surprisingly, the up-converted signal of $BP(OH)_2$ inside the CB7 nano-cavity does not exhibit any growth component characteristic of two-step sequential process. Interestingly, the growth component exists inside the nano-cavity of β-CD (having similar cavity size as that of CB7), infering the presence of two-step sequential process of PT inside the β-CD nano-cavity. The different features of PT dynamics of $BP(OH)_2$ in the above mentioned two macrocyclic hosts may be attributed to the presence and absence of water solvation network surrounding the $BP(OH)_2$ inside the nano-cavities of β-CD and CB7, respectively.

Bio-molecular and Material Interactions

In-vitro probing of protein-DNA interaction is monitored by fluorescence switching of an eminent anti-cancer drug, ellipticine. It is observed that fluorescence switching takes place from blue to green when serum albumin (SA)-bound ellipticine interacts with DNA.



Electron microscopic (SEM) images disclose the existence of radially branched dendritic architecture in protein-DNA system where DNA starts nucleation at the tip of 'fern leaf' aggregates of protein. We believe this simple but effective strategy of using visible colour switch as a tool to monitor protein-DNA interaction will be helpful in understanding many important cellular processes in vitro and in vivo.

Graphene oxide based molecular switching of ellipticine (E) has been utilized to probe its efficient loading onto graphene oxide (GO) and subsequent release to intra-cellular biomolecules like DNA/RNA. The green fluorescence of E switches to blue in GO and switches back to green by polynucleotides. The intensified blue emission of the ellipticine-GO (E-GO) complex with human serum albumin (HSA), switches to bluish green upon addition of dsDNA. Electron microscopy reveals the formation of distinctive 3D assemblies involving GO and biomolecule(s) probably through non-covalent interactions and is primarily responsible for the biomolcule(s) assisted fluorescence-switching of E. To our knowledge, such morphological pattern of GO-DNA complex is very unusual, reported here the first time and could find applications in the fabrication of biomedical devices.

In future, his group will try to understand the water dynamics in A-DNA, Z-DNA and RNA. They will also focus the interaction features of different biomolecules and graphene, considering biomedical applications of graphene and its derivatives. The group is also interested to build-up fluorescence lifetime correlation spectroscopic technique in order to understand many important biological events, e.g. DNA compaction process in single molecular level. The dynamics of flavoprotein will be explored using transient absorption and transient grating techniques.

Structure and dynamics in the function of biomolecules

Fast, local motion in enzymes

A major goal of **Puranik's** laboratory is the elucidation of the role thar fast, local motions play in enzyme catalysis. Proteins are flexible structures with dynamics on many different time-scales from femto- to milli-seconds. Understanding the role of these dynamics in protein function is a major goal in the field of enzymatic catalysis. Slower motion (us-ms) is now understood to be important for creating catalytically active conformations and controlling the access of small molecule substrates to the active-site. Motion relevant to chemistry at the active-site is at faster, femtosecond (fs) timescales. There are only a handful of studies that have examined protein motion on this fast timescale. **Puranik's** group aims to understand structural and electronic changes in the substrates due to protein environment and the role of fast dynamics at the active-site relevant to catalysis. Some of the questions being addressed are: **what is the timescale and magnitude of response of the enzyme active-site to excitation of bound ligands? Do allosteric effectors influence fast dynamics at the active-site? Do site mutations remote from the active-site influence these dynamics? In analogus proteins from different organisms, does protein dynamics contribute to differential catalytic abilities?**

Dynamics of molecules

Puranik's laboratory has measured the excited state dynamics, intramolecular relaxation and reactivity of nucleic acids and aminoacids. Experimental measurements of direct time-resolved femtosecond vibrational spectra at <100 fs is not possible because the uncertainty principle leads to a large spectral width for short pulse duration. This is overcome by making experimental measurements of spectral broading followed by wave-packet dynamical modeling of the experimental measurements. Her group has observed an ultrafast (<100fs) component of Trp relaxation dynamics for the first time and shown that both, inter and intra-molecular relaxation occurs on this time-scale.

Raman measurements and TDDFT calculations on several purines – adenine, 2-aminopurine and 2,6-diaminopurine have lead to an understanding of how location of the amino-group influences the relative ordering of excited states.

Dynamics inside the protein core

The timescale and magnitude of residue dynamics in the core of natively folded protein, Barstar[3,4] was determined. This was accomplished by using a buried tryptophan residue as a probe. **A first example of a CH-pi interaction at the core of a protein was identified.** Unique signature of this CH-pi interaction was used to follow the kinetics of core assembly, water exclusion and consolidation during folding. This permitted the delineation of steps in the core assembly not observable with traditional methods.

Protein-ligand interactions

Puranik's group is studying the function and dynamics of nucleic acid binding enzymes from DNA repair and purine salvage pathways in terms of the enzyme's ability to recognize multiple substrates while still retaining specificity of the chemical catalysis step. Some of the enzymes are: Fpg of the Base Excision Repair pathway; an in-situ DNA repair demethylase, AlkB; and purine recycling pathway enzymes (HGPRT and ADSS) that are being studied using molecular biology and spectroscopic studies.

In HGPRT, an enzyme that converts free nucleobases into corresponding nucleotides, it was shown that the enzyme distorts bound nucleobases upon binding with differential extent of distortion for different substrates. Using non-cleavable substrate analogues it was shown that despite 80% identity in their active-sites, human and malarial parasite (Plasmodium falciparum) enzymes have differential ability to bind, distort and catalyse common substrates.

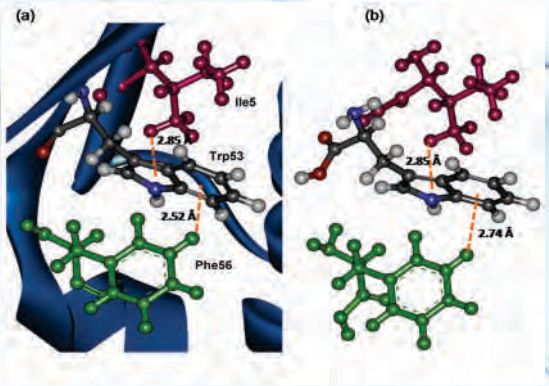


Figure shows the CH-pi interactions between a tryptophan, phenylanaline and isoleucine residues in the core of a native, folder strcture of Barstar protein.

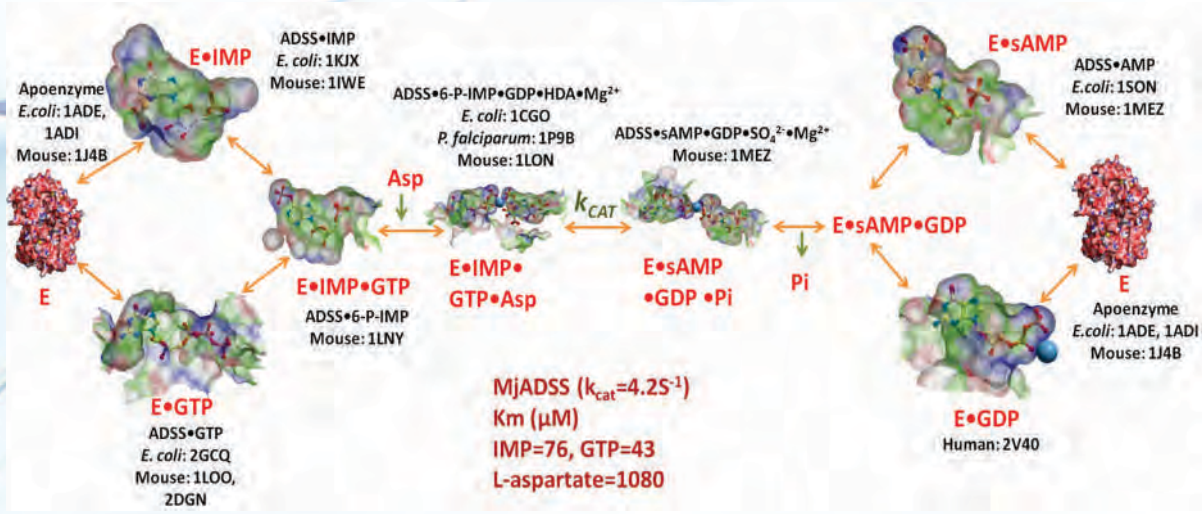


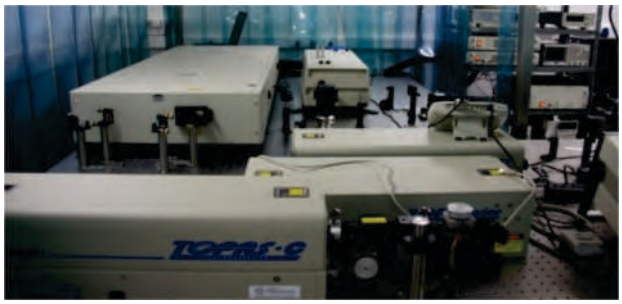
Figure illustrates the kinetic cycle of ADSS showing ordered binding of several substrates. Each enzyme-substrate complex is being examined with ultraviolet resonance Raman spectroscopy using our home-built instrument.

Adenylosuccinate synthetase (ADSS), which has multiple substrates, is a more complex system. IMP, GTP and L-asp bind to ADSS to produce adenylate succinate. The allosteric influence of GTP on IMP, is being examined. Complexes of the enzyme with various substrates are being studied with an aim to detect transient intermediates and understand the origin of directional kinetics of this enzyme.

Dynamics of a substrate bound within the active-site of an enzyme

The future plans are to measure the femtosecond dynamical coupling between a nucleotide substrate and human HGPRT enzyme to understand the role of fast, local motions in assisting the chemical step of conversion of substrates to products.

Terahertz spectroscopy

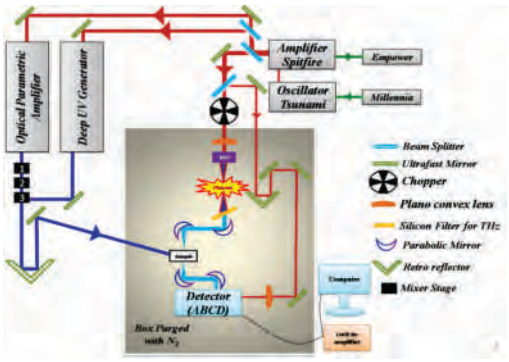


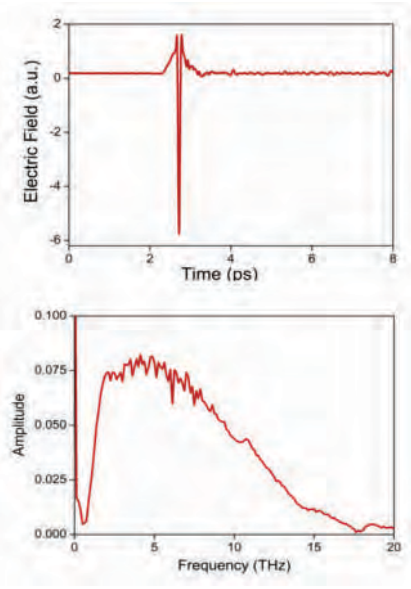
Pankaj Mandal is exploring the "Terahertz (THz) gap" in the electromagnetic spectrum, which became accessible only recently and opens new avenues of probing matter at ultrafast time scales and at the nanoscale. THz frequencies, typically 0.1 to 15 THz (3 to 500 cm^{-1}), span the range of low-energy excitations in electronic materials, low-frequency vibrational modes of condensed phase media, and vibrational and rotational transitions in molecules. Hence this is a key spectral range for probing fundamental physical interactions as well as practical applications with great technological promise for security and medical imaging. Specifically, time-resolved THz spectroscopy is being used to study the carrier and spin dynamics in nanoparticles and hydrogen-bond dynamics in solvated biomolecules.

THz spectroscopy is 'the ideal' technique to probe the above dynamical processes because the time scales related to them are in the picoseconds (10^{-12}) range which corresponds to THz frequency (10^{12} Hz).

Pankaj Mandal's group has built high power large bandwidth THz spectrometer at IISER-Pune. Broadband THz pulse of sub-picosecond duration is produced from a four-wave-mixing process in air-plasma created by amplified ultrafast laser pulse. This method of generation of THz radiation produces very large bandwidth, limited only by the pulse width of the laser light used. They have successfully implemented "Air Biased Coherent Detection" scheme for detecting large bandwidth THz light. A bandwidth of ~18 THz has been achieved. Such set-up for carrying out ultra

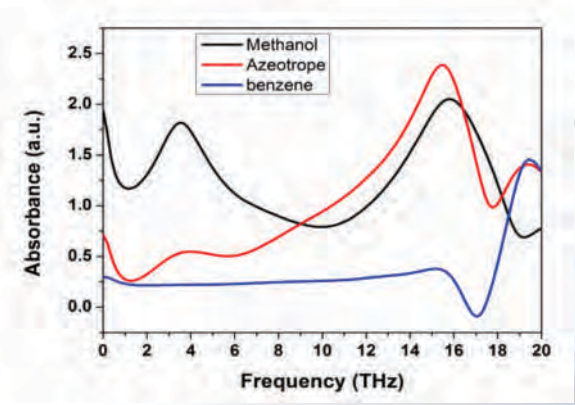
broadband THz spectroscopy is available only in few laboratories in the whole world, and is built for the first time in India. An experimental set-up for "optical pump-THz/whight light probe Spectroscopy" has already been built. This set-up will enable probing a time-dependent (transient) event using either a broadband THz or a broadband white light (WL) as probe. A temporal resolution of 50 femto-second (fs) can be achieved.

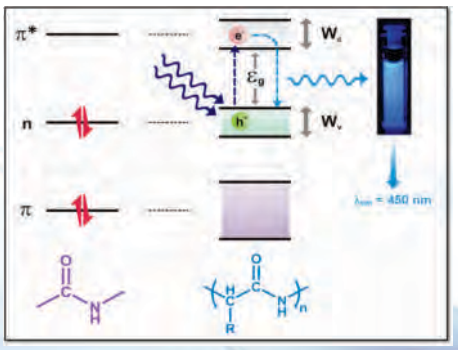




Currently the following problems are of interest to the group: 1) Probing multiple exciton generation (MEG), carrier dynamics, phonon dynamics in semiconductor nanocrystals, 2) THz induced magnetization dynamics in magnetic naomaterials and molecular magnets, 3) Hydrogen-bond dynamics, solvation dynamics in liquid water and water-biomolecule network, and 4) intermolecular interactions and related dynamics in binary/ternary liquid mixtures.

Mandal's group have studied THz spectroscopy and molecular dynamics simulation (in collaboration with Dr. Arnab Mukherjee) of methanol-benzene azeotrope and trying to evaluate the delicate balance of intermolecular interactions between molecules involved which lead to the formation of azeotropic mixture. Their finding indicates towards a first-order liquid/liquid phase transition from a non-azeotrope to an azeotropic mixture at elevated temperature.





Unusual blue-green emission has been observed in amyloid fibril, crystalline protein and in protein solutions. Often protein aggregation is attributed to this unusual visible emission. However, the origin of this emission is not known exactly. Dr. Mandal's (in collaboration with Dr. P Hazra) spectroscopic studies of serum proteins revealed that blue-green emission is, most likely, a property of protein monomer. Evidences suggest that semiconductor-like band structure of proteins with the optical band-gap in the visible region is possibly the origin of this phenomenon. They have shown that the band structure of proteins is primarily the result of electron delocalization through the peptide chain, rather than through the hydrogen bond network in secondary structure.

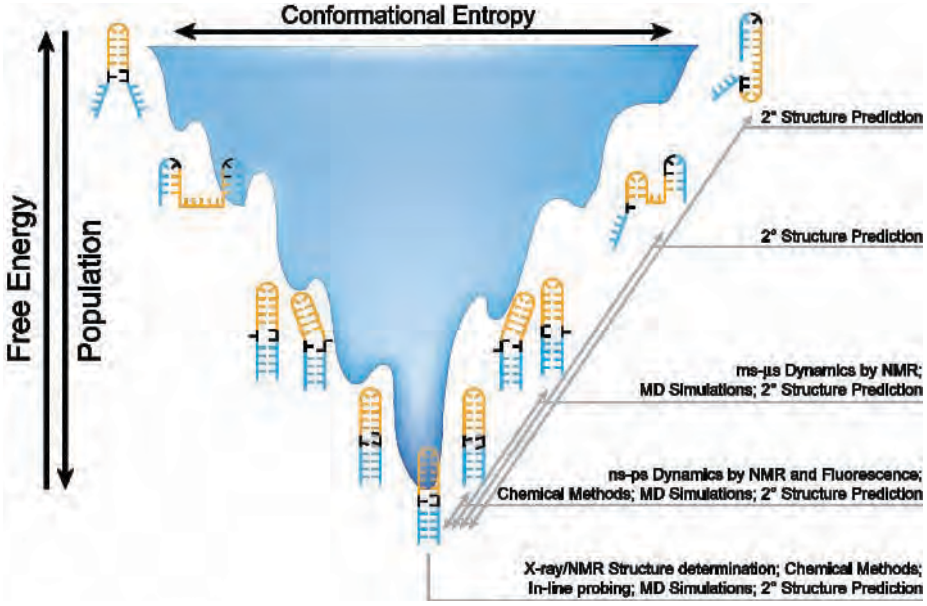
Matrix isolation THz spectroscopy: The intermolecular interactions such as hydrogen bonding, pi-pi interaction, van der Waals interactions etc between molecules are very important in condensed phase. The intermolecular vibrations have frequencies in the THz range. In addition to study of these intermolecular forces in condensed media,

understanding their nature in isolated molecular complexes will provide more detailed and clear fundamental picture about them. Dr. Mandal's group is planning to combine their THz spectrometer with Matrix Isolation technique to study different weakly bound complexes between molecules trapped in matrix of inert gas. This will be the very first such experimental technique to study the intermolecular interactions directly.

Biomolecular NMR Spectroscopy

The main research focus of **Jeetender Chugh's** group is on various aspects of solution NMR including theoretical design and experimental implementation of new NMR experiments to probe the biophysical characteristics of RNA and proteins; understanding functional aspects of non-coding RNAs; and structural biology of microRNAs and their regulation in various disease settings.

ms-μs dynamics in RNA With the current plethora of structure prediction algorithms, it is possible to predict sub-optimal secondary structures for a given RNA sequence. However, the number of these sub-optimal secondary structures, as predicted by various structure prediction algorithms available, increases exponentially both with increase in the number of nucleotides in the RNA sequence and with increase in the energy range. Although, for small RNAs and for small energy range these algorithms do pretty well, but still there is a need to validate these 'feasible' structures experimentally. Experimental characterization of alternative structures for small RNAs using state-of-the-art R1 NMR relaxation dispersion experiments has been done successfully but is a time consuming and expensive affair. Thus there is a dire need to formulate sequence codes that would predispose the sequence towards such motions and allow predicting precise sub-optimal secondary structures without the need of experiments.



miRNA biogenesis pathway

All miRNAs do not follow a universal pathway for their biogenesis. Specific mechanisms in the biogenesis of individual class of miRNAs suggest multiple opportunities for tight regulation of miRNA levels. This spectrum of distinct mechanisms is widening everyday as more and more interacting partners are being identified. Although several reports emphasize on the regulatory activities of miRNAs, very little is known about the structural (primary, secondary or tertiary) understanding of the regulation of miRNA expression levels and their activity. Therefore, understanding the conformational roles fundamental for these regulatory mechanisms in the miRNA biogenesis pathway may act as a path-breaking step for development of new drugs based on RNAi mechanism.

D. Spectroscopy and Dynamics

Computational Chemistry

Arun Venkatnathan's group focuses on the application of quantum chemistry methods and Molecular Dynamics (MD) simulation to characterize molecular and nano-scale properties of materials of relevance to alternate energy. Specific problems of interest are the nanostructure and molecular transport of polymer electrolyte membranes under various fuel cell operating conditions; spectral properties and energetics of various clathrate hydrates; proton transport and nano-scale behaviour of imidazolium ionic liquids.

Molecular Simulation of Polymer Electrolyte Membranes

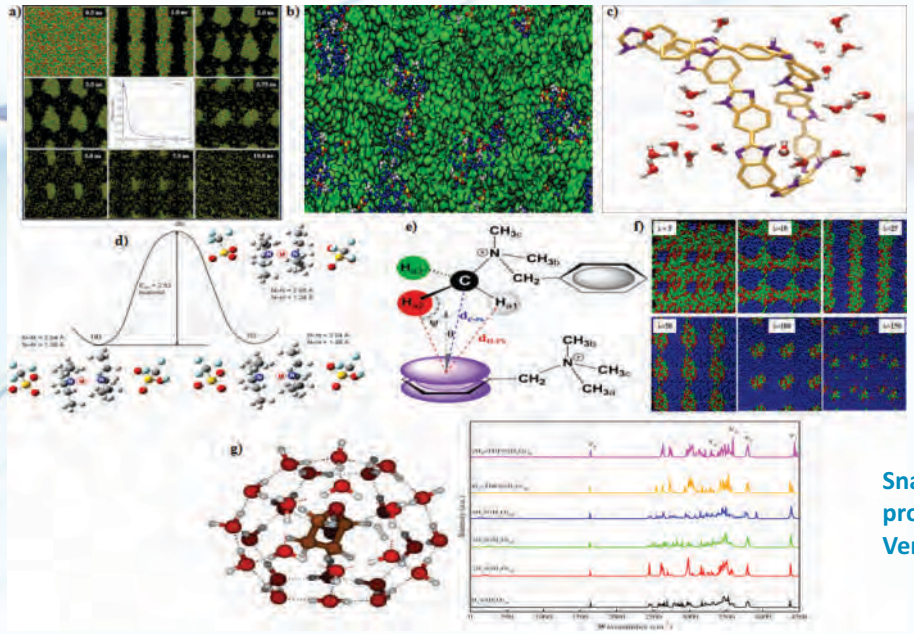
Polymer Electrolyte Membrane (PEM) fuel cells offer strong potential for delivering power with high efficiency and minimal emissions making it an attractive choice for stationary and portable applications. The polymer membrane acts like an electrolyte and is responsible for proton conduction. Some of the important contributions and findings from Arun Venkatnathan's group are: development of force-field parameters for triflic acid and triflate ion as proton conducing groups (Fig. a), simulation of side chain pendants of various Perfluorosulfonic acid polymer membranes to illustrate their influence on structure and dynamics of hydronium ion and water transport, examination of nanostructure (Fig. b) of Aciplex polymer membrane and molecular transport (at varying hydration and temperature) and comparison with Nafion. The group has performed detailed analysis on various interactions and dynamical properties of benzimidazole (monomer and polymer) membranes with phosphoric acid and triflic acid and examined the effect of polymer chain length, phosphoric acid concentration and temperature. The simulations predict that the decamer of the ABPBI membrane (Fig. c) is the optimum polymer chain length beyond which no significant change in properties is observed. The blend of phosphoric acid and triflic acid doped with ABPBI membrane could be the most effective in reducing acid leaching from the membrane matrix.

Proton transport and nano-scale behavior of Ionic Liquids

Arun Venkatnathan's group has examined proton-transport pathways in a triethylammonium-triflate (TEATF) ionic liquid (IL)-doped side chain of a polymer electrolyte membrane using quantum chemistry calculations. The calculations (Fig. d) predict that proton transfer from a tertiary amine cation ($TEAH^+$) to a tertiary amine (TEA) occurs only with an interaction with an anion (TFA^-), which increases its basicity. Results have a bearing on the experimental choice of IL to provide enhanced proton conduction in polymer electrolyte membrane environments. The group has also characterized the structure and dynamics of Ammonium based benzyl-NX_3 (X=Methyl, Ethyl) trifluoromethane-sulfonate ILs using MD simulations and ionic conductivity using Electro-chemical Impedance Spectroscopy (EIS) at varying temperature and Relative Humidity (RH). The BzTMA cations show both C-H/Ph and cation-Ph interactions, whereas BzTEA cations show only strong cation-Ph interactions (Fig. e). Further, the group has explored the effect of water concentrations on structure of hydrophobic imidazolium IL and have observed phase-segregation (Fig. f), cationic tail aggregation and micelle formation. The results from this work provide a molecular understanding of influence of water on properties of such ILs used in various technological applications.

Clathrate Hydrate Chemistry

Arun Venkatnathan's group has also examined the structure, stability and spectral properties of clathrate hydrates (lattice formed from various water cages) using Density Functional Theory. The calculations performed using dispersion included functionals accurately predict spectral properties of encapsulated methane and hydrogen molecules in various water cages and are consistent with experiments performed on the hydrate lattice. The maximum occupancy and calculated spectra (Fig. g) of hydrogen occupied cages (with and without Tetrahydrofuran dopant) validate the observations on characterization of hydrogen storage done by several experiments.



Snapshots of some research projects in Arun Venkatnathan's group.

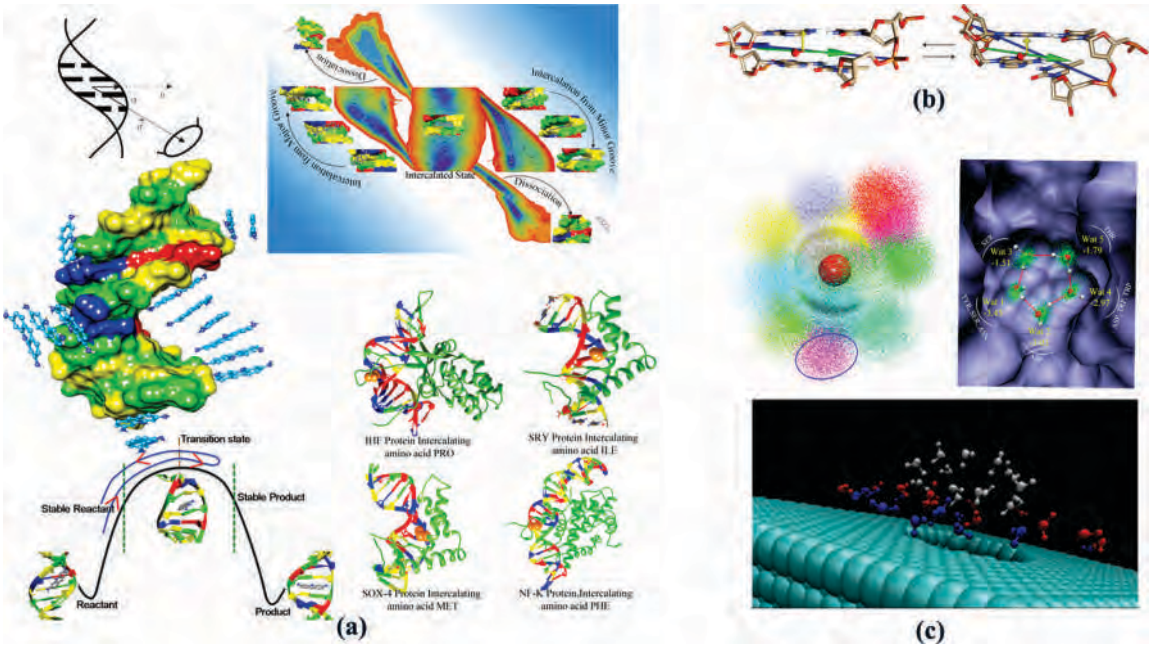
Future directions

Arun Venkatnathan's group will examine anionic size effects, variation in alkyl chain length of the imidazolium cation and influence of temperature on the nanostructure and dynamics of several imidazolium ILs. Such a molecular level understanding can assist in choice of ILs for various applications like electrolytes, CO_2 capture etc. The group also aims to investigate proton transport in imidazole chains using gas-phase quantum chemistry calculations and characterize properties of binary IL mixtures and IL doped PEM (for anhydrous proton conduction) using MD simulations.

Computational Biophysics

Research activities of **Arnab Mukherjee's** group (AMG) focuses on the molecular mechanism and thermodynamics of biological recognition processes, conformational transitions, etc. Each member of the group works in different areas involving drug-DNA and protein-DNA intercalations, enzymatic activity, DNA structural transition, role of water, etc. Simultaneously, fundamental research interest on various topics of physical chemistry, e.g., azeotropic mixture, chaotropic mixtures, even simple water are also of group's interest. Their group collaborates with experimental groups often to provide a molecular understanding to observed phenomena with the help of detailed molecular dynamics simulation. Some of the details are mentioned briefly below. A snapshot of some of the projects running in the group is given in the following figure.

Mechanism of Intercalation of Anti-cancer Drugs to DNA Intercalation of drug into DNA is the first step towards the mechanism of anti-cancer activity by anthracycline antibiotics. AMG has shown for the first time the molecular mechanism of intercalation of drugs into DNA using an anti-cancer agent proflavine. Using a designed reaction coordinate (Fig. a), they showed that the process goes via a minimal base-stacking penalty pathway. Also, the detailed free energetic studies carried out by their group shows that the drugs bind to the minor groove first before intercalating through major groove (Fig. b). This pathway gives the timescale of the process similar to what is observed in experiment. Direct intercalation through minor or major will lead to much longer (seconds) and shorter (microsecond) timescale. They also showed that the binding of the proflavine (Fig. c) to DNA is much faster (nanosecond) compared to reported experimental estimate from fluorescence kinetic studies (sub-millisecond). AMG is currently exploring the dynamical effect (recrossing and internal friction) of the process near transition state (Fig. d). Another continuation of the intercalation project is to study the mechanism of kink formation in DNA by



intercalation of amino acids of the bound protein, typically observed in transcription factors (Fig. e). AMG has found that the partial intercalation of amino acid is responsible for kink formation.

DNA Structural Transition and application in Nanodevices DNA is polymorphic by nature. Depending on the external environment, DNA can take different conformations known as B-DNA, A-DNA, Z-DNA, etc. Structural transition in DNA has been exploited in devices as well. There have been numerous studies on the structural transition of the DNA from B- to A-form. However, AMG was the first to calculate the structural change at a local dinucleotide level. They introduced a new dynamical coordinate Zp' (Fig. f) to calculate the free energy change required for converting a dinucleotide step from B- to A-form. Thereby, they captured the propensity of A- and B- form for all the different dinucleotides. Their calculations also revealed that the creation of a local dinucleotide gives rise to a penalty in terms of B/A junctions. Subsequently, they formulated a model to predict DNA conformation based on the absolute free energy change for a dinucleotide step from B- to A-form. They are currently working towards the goal to see whether the transition is nucleation driven and what the role of sequence dependence is. In continuation, AMG is working on DNA translocation through graphene nanopore. The objective is to study whether the structure of DNA has any role in translocation.

Single Water Entropy and its application in drug design It is known that when two species bind together in water, some water molecules go to the bulk. This process results in the increases in overall entropy of the system, thereby stabilizing the bound state. Significant effort in drug discovery focussed to find the low entropy water bound to the active site so that a particular drug can be designed to replace those making the bound complex free energetically stable.

AMG used permutation reduction approach (Fig. g) to calculate the entropy of a single water molecule around a bimolecular species. They showed that even in a particular protein cavity, water molecules possess different entropy (Fig. h). They also showed how the entropy of water changes as a function of distance from the particle. They are applying this method in various other systems such as hydrophobic and hydrophilic cavity (Fig. 1i), amino acids, DNA, etc.

Other Projects There are various other projects running in **Arnab Mukherjee's** group. Some of the projects worth mention are collaborative in nature. With Dr. Partha Hazra, AMG has worked on the effect of urea in FAD conformation. With Dr. Pinaki Talukdar's group, AMG has worked on the molecular picture of Cl- ion translocation through a synthetic ion channel (Fig. j). With Dr. Pankaj Mandal's group, AMG is currently pursuing the structural, dynamical and spectroscopic signature of an azeotropic mixture (Fig. k).

Future Directions Arnab Mukherjee's group has made a significant advancement in the area of drug-DNA intercalation. Their group is going to extend their work towards protein-DNA, drug-RNA intercalation. The future goal of the group is to work on drug discovery where their work on entropy of a single water molecule will be useful. Combining this approach with the work on DNA nano-devices, AMG group aims to take their research towards the general direction of nano-medicine.

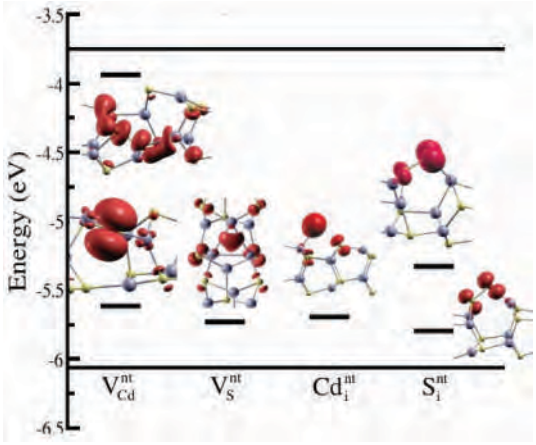
Computational Material Science

Prasenjit Ghosh's group is interested in (a) understanding aspects of chemical bonding and microscopic couplings that are essential to the specific properties of materials, (b) obtain information about atomistic structure and electronic states which are often hard and sometimes inaccessible to experiments and (c) in silico design of new materials and/or modification of the existing materials to yield new materials with desired properties. His group achieves this by performing first principles calculations using quantum mechanical density functional theory (DFT) and density functional perturbation theory (DFPT). The excited state properties are studied by time-dependent density functional theory (TDDFT). Currently his group is interested in materials, which are of importance in heterogeneous catalysis, photocatalytic water splitting, photovoltaics and thermoelectrics. Further his group is also interested in exploring the physics and chemistry of low dimensional materials. Given below are some examples of ongoing projects in his group:

(a) Heterogeneous catalysis

Selective hydrogenation of acetylene to ethylene is an important chemical reaction. The catalyst used for this reaction should exhibit not only high reactivity but also high selectivity. The latter is necessary to prevent complete hydrogenation of acetylene to ethane. Pd is currently used as a catalyst in this reaction. However, Pd catalysts exhibit poor selectivity. In an effort to design new catalysts for this reaction, Prasenjit Ghosh's group used sub-nanometer bimetallic PdGa clusters in gas phase and studied the catalytic activity of these clusters for the above mentioned reaction. They found that though Pd_3Ga clusters show high reactivity, they are not selective. However, Pd_2Ga_2 clusters show large selectivity with reactivity slightly lower than the Pd_3Ga clusters. For practical applications, the clusters are deposited on oxide supports. Presently their group is investigating the growth and formation of these clusters on MgO (a commonly used support). Further they are also investigating how the support effects the reactivity and selectivity of these clusters.

(b) Role of defects in the optical properties on CdS nanotubes

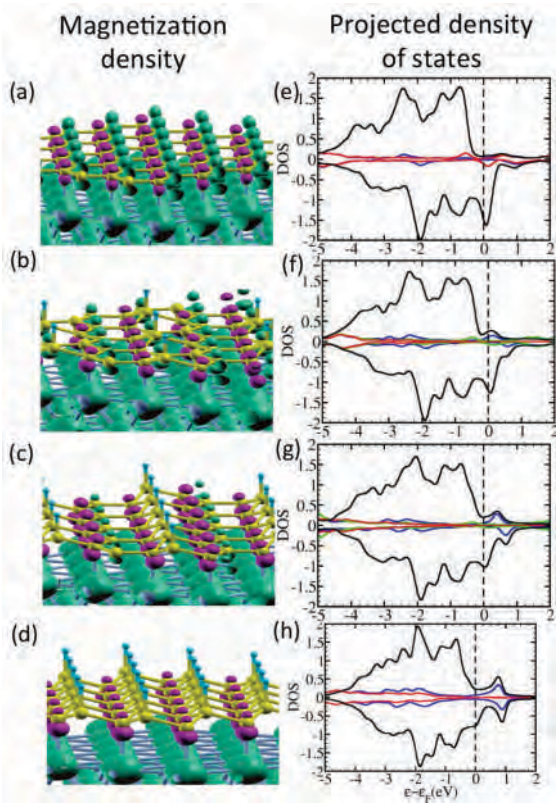


CdS nanostructures are prospective candidates for designing semiconductor based solar cells. However, during the growth process, several defects are found in these materials which significantly alter their optical properties. In collaboration with Dr. Shouvik Datta's group, Prasenjit Ghosh's group investigated the absorbance and photoluminescence properties of cadmium sulphide nanotubes with overall size beyond the quantum confinement regime. The experiments performed in Dr. Datta's group showed that while the absorption spectra are unaffected by the change in size of the nanotubes, there is an anomolous red shift in their photoluminescence spectra with increase in their size. With the help of density functional theory calculations performed by Prasenjit Ghosh's group, they have identified that the shift in the emission peak of the photoluminescence spectra is a result of the interplay between Cd vacancies on the surface of these nanotubes and the crystalline strain, which was incorporated in these nanotubes during their growth process. Most importantly the calculations show that rather than the defect concentration, it is the nature of the defect, which plays a crucial role in determining the optical properties of these nanotubes. For this particular case

of CdS nanotubes it has been found that though S interstitials are the most abundant defects, it is the Cd vacancies with second lowest formation energies which significantly affect the photoluminesence spectra.

(c) Hydrogen induced spin reversal in graphene supported on Ni(111) surfaces

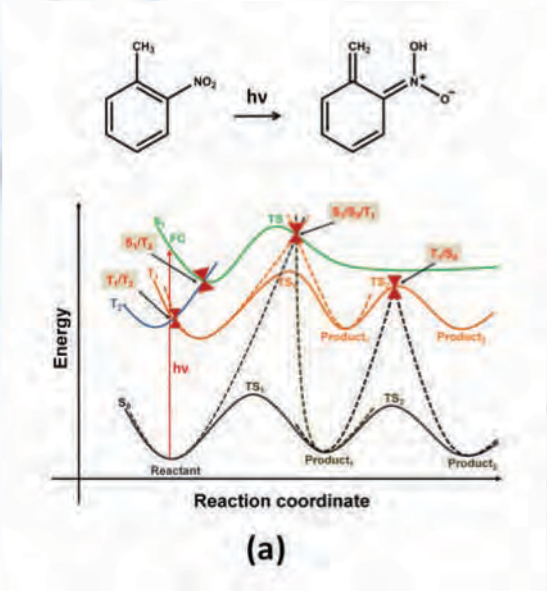
Prasenjit Ghosh's group presents a novel way of changing the alignment of the induced magnetic moment of graphene supported on Ni(111) surface through hydrogenation. For the pristine graphene on Ni(111) surface, the magnetic moments on the fcc (top) C atoms are parallel (anti-parallel) with respect to those of the Ni atoms. The graphene sheet becomes ferrimagnetic with the average magnetic moment of the graphene sheet parallel with respect to that of the Ni atoms of the substrate. Through density functional theory based study, they show that this alignment can be controlled upon gradually hydrogenating the supported graphene layer. At maximum H coverage (0.5 ML), they find the supported hydrogenated graphene to be a ferromagnetic semiconductor, the average magnetic moment of the graphene sheet is anti-parallel with respect to the Ni atoms. Preliminary studies suggest that the hydrogenated graphene sheet can act as a tunneling barrier for magnetic tunnel junctions.



In summary, Prasenjit Ghosh's group, using *ab initio* DFT has been able to identify sub-nanometer catalyts for different important industrial reactions, understand the role of defects in altering the electronic structure of materials and their effect on the optical properties. They have also been able to understand different important and novel physical and chemical properties in layered structures. This knowledge will provide valuable guidelines for experimentalists to synthesize new materials with desired properties.

Photoinduced Molecular Processes

Research in **Anirban Hazra**'s group focuses on studying excited state molecular phenomena. The emphasis is on understanding mechanism of such phenomena using tools from electronic structure theory and nonadiabatic dynamics. Several of these processes like photoinduced electron transfer, photodissociation and florescence quenching occur at the ultrafast or femtosecond timescale and play important roles in living organisms and in atmospheric processes. The detailed mechanistic understanding, that the group's research seeks, is of basic scientific interest and is also important for its technological implications in solar-based renewable energy devices, particularly the conversion of solar energy to chemical energy. There are several projects going on in the group currently.

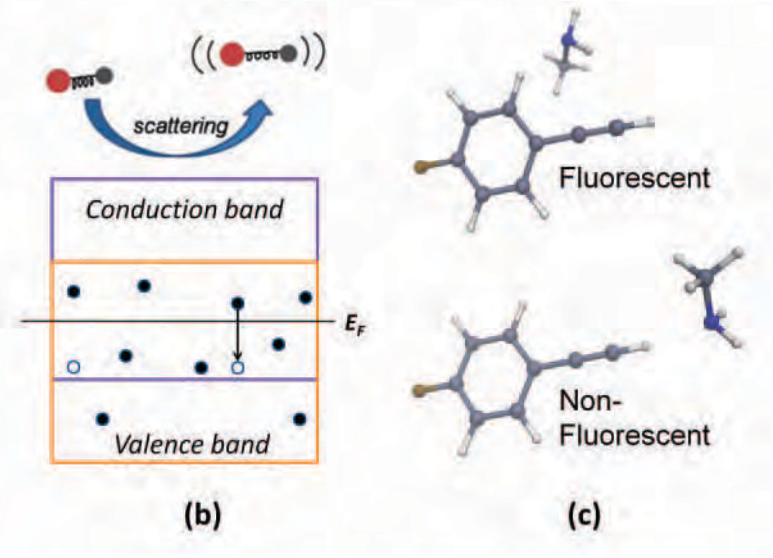


Excited-state hydrogen transfer (ESHT) is a reaction with major chemical and biological significance. The mechanism of

an ESHT reaction leading to tautomerization of *o*-nitro toluene to its aci-nitro tautomer is being investigated. The reaction is found to proceed through a complex pathway, involving both singlet and triplet states. There are interesting topological features on the potential energy surfaces like two and three-state conical intersections that have been identified, and which are important for the reaction dynamics. A method to find three-state conical intersections has been developed and implemented.

Accurate modeling of nonadiabatic energy transfer during scattering of molecules from metal surfaces has been a challenge due to the large number of metal electrons that need to be included in the model for realistic simulations, which makes the quantum mechanical propagation of the wavefunction computationally very demanding. Few years back, a method called independent-electron surface hopping was proposed by Shenvi, Roy and Tully (J. Chem. Phys., 130, 174107 (2009)), that provides an approximate way to treat such systems. This method is being implemented and will be applied to to explain energy transfer to intra-molecular degrees of freedom during scattering of molecules from surfaces.

It has been recently observed through gas phase laser spectroscopy (by our experimental collaborators) that there exist at least two stable conformers for the weakly-bonded complex between fluorophenylacetylene (FPHA) and methylamine. It was found that one of the conformers was fluorescent while the other was not. Such a dramatic change to the optical properties due to a conformational difference, dictated by weak interactions, is intriguing. The mechanism for this phenomenon is being explored using the complete active space self-consistent field (CASSCF) electronic structure calculations. The presence of conical intersections and large vibronic coupling between states are hypothesized to cause the quenching of fluorescence, and this is being tested.

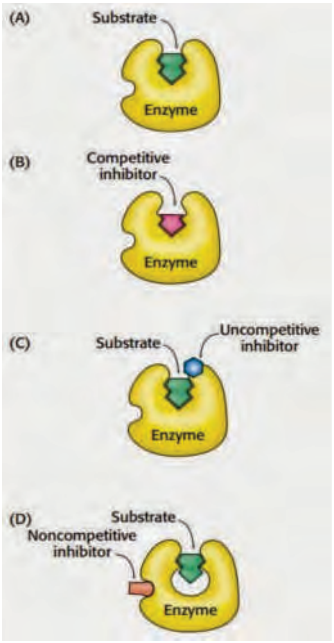


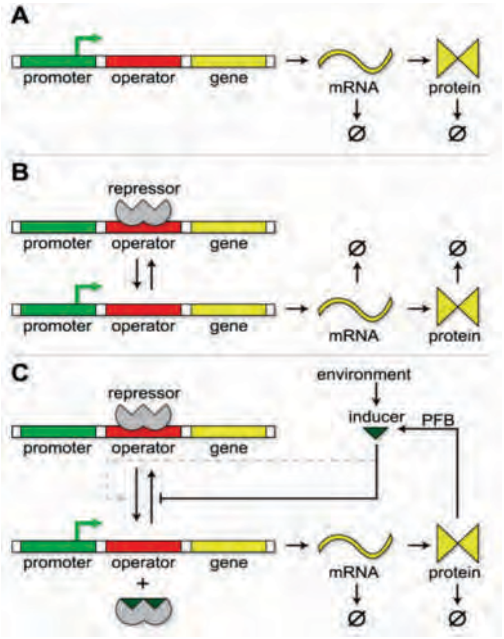
The research in Anirban Hazra's group covers a diverse range of chemical phenomena involving excited states. Due to advances in spectroscopic techniques in recent decades, there is a huge amount of experimental data available on excited states, but the theory to interpret this is relatively nascent. The group sees this as an exciting opportunity and plans to continue contributing to the development of methods to understand excited state processes.

Stochastic Processes

Srabanti Chaudhury and her group is interested in developing theoretical models based on the principles of time dependent statistical mechanics and apply them to understand interesting problems in chemical physics, biological physics and soft condensed matter. Her group is actively investigating biological processes at the cellular level in which randomness and stochasticity play an important role and how the stochasticity that is inherent in its dynamics can be characterized and treated mathematically.

Understanding the interconnection between the specificity of an enzyme, the architecture of the active site and the kinetic mechanism of a reaction are of major importance. In one of the group's recent work, she investigates the role of stochastic fluctuations in single molecule enzyme inhibition kinetics. The various ways in which these inhibitors can bind to the enzyme in competition with the substrate and mask the catalytic activity of the enzyme is important to





investigate as it could provide insight for designing inhibitors specific to certain enzymes/drugs. Srabanti Chaudhury has proposed a stochastic model that can be predictively utilized to successfully distinguish between different types of inhibition reactions types mechanisms depending upon the binding site of the enzyme.

Srabanti Chaudhury's group is working on understanding the role of stochastic fluctuations in mRNA levels on gene expression. They have proposed a new theoretical method to study the dynamics of switching in a two state gene expression model by explicitly accounting for the transcriptional noise. Analytical predictions are being tested with Monte Carlo simulations and experimental observations.

In summary, Srabanti Chaudhury's research mainly involves the development of analytical tools to study a wide variety of biological systems. Her analytical work is extremely challenging and is properly complemented with simulations and available experimental results.

In future, apart from modeling enzymes, Srabanti Chaudhury's group is also keen on modeling the catalytic activity of metal nanoparticles. Owing to their heterogeneous distribution of surface active sites and availability of two concurrent product dissociation pathways, it is challenging to model such systems theoretically. Srabanti's group is also interested in understanding the role of protein pore interactions for translocation of polypeptides through nanopores. This work would involve theoretical modeling as well as detailed molecular dynamics simulations.

Chemistry Publications

1 Kumar V. A.; **Ganesh K. N.** Structure-Editing of Nucleic Acids for Selective Targeting of RNA, *Curr. Top. Med. Chem.* **2007,** 7, 715-726.

2 Patwa, A. N.; Gupta, S.; Gonnade, R. G.; Kumar, V. A.; Bhadbhade, M. M.; **Ganesh, K. N.** Ferrocene-Linked Thymine/Uracil Conjugtes: Base pairing Directed Self-Assembly and Supramolecular Packing. *J. Org. Chem.* **2008,** *73*, 1508-1515.

3 Purbey, P. K.; Singh, S.; Pavan Kumar, P.; Mehta, S.; **Ganesh, K. N.;** Mitra, D.; Galande, S. PDZ domain-mediated dimerization and homeodomain-directed specificity are required for high-affinity DNA binding by SATB1. *Nucleic Acids Res.* **2008,** 7, 2107-2122.

4 Vysabhattar, R.; **Ganesh, K. N.** Cyanuryl peptide nucleic acid: synthesis and DNA complexation properties. *Tetrahedron Lett.* **2008,** 49, 1314-1318.

5 Patwa, A. N.; Gupta, S.; Gonnade, R. G.; Kumar, V. A.; Bhadbhade, M. M.; **Ganesh, K.N.** Ferrocene-Linked Thymine/Uracil Conjugates: Base pairing Directed Self-Assembly and Supramolecular Packing. *N. J. Org. Chem.* **2008,** 73, 1508-1515.

6 Anilkumar, P.; **Jayakannan, M.** Divergent Nanostructures from Identical Ingredients: Unique Amphiphilic Micelle Template for Polyaniline Nanofibers, Tubes, Rods and Spheres. *Macromolecules* **2008**, *41*, 7706-7715.

7 Anilkumar, P.; **Jayakannan, M.** Hydroxyl Functionalized Polyaniline Nano-spheres: Tracing Molecular Interactions at Nano-surface via Vitamin-C Sensing. *Langmuir* **2008**, *24*, 9754-9762.

8 Amrutha, S. R.; **Jayakannan, M.** Probing the π-stack Induced Molecular Aggregation in π-Conjugated Polymers, Oligomers and Their Blends of Poly(phenylenevinylene)s. *J. Phys. Chem. B* **2008**, *112*, 1119-1129.

9 Deepa, P.; **Jayakannan, M.** Polyurethane-Oligophenylenevinylene Random Copolymers: π-Conjugated Pores, Vesicles and Nano-Spheres via Solvent Induced Self-organization. *J. Polym. Sci. Polym. Chem.* **2008**, *46*, 5897-5915.

10 Deepa, P.; **Jayakannan, M.** Solvent Free and Non-isocyanate Melt Transurethane Reaction for Aliphatic Polyurethanes and Mechanistic Aspects. *J. Polym. Sci. Polym. Chem.* **2008**, *46*, 2445-2458.

11 Anish, C.; Amrutha, S. R.; **Jayakanann, M.** Renewable Resource based Poly(m-phenylenevinylene) and their Statistical Copolymers: Synthesis, Characterization and Probing of Molecular Aggregation and Forster Energy Transfer Processes. *J. Polym. Sci. Polym. Chem.* **2008**, *46*, 3241-3256.

12 Reddy J. S.; **Anand V. G.** Conjugated Macrocycles from Thiophenes and Benzenes. *Chem. Commun.* **2008**, 1326.

13 Reddy J. S.; **Anand V. G.** Planar *Meso* Pentafluorophenyl Core Modified Isophlorins. *J. Am. Chem. Soc.* **2008**, *130*, 3718.

14 Balamurugan, A.; Reddy, M. L. P.; **Jayakannan, M.** Single polymer Photosensitizer for Tb3+ and Eu3+ ions: A Novel Approach for White Light Emission based on Carboxylic Functionalized poly(m-phenylenevinylene)s. *J. Phys. Chem. B* **2009**, *113*, 14128-14138.

15 Anilkumar, P.; **Jayakannan, M.** Self-assembled Cylindrical and Vesicular Molecular Templates for Polyaniline Nanofibers and Nanotapes. *J. Phys. Chem. B* **2009**, *113*, 11614-11624.

16 Amrutha, S. R.; **Jayakannan, M.** Supramolecular Ring Banded Prototype Liquid Crystalline Oligo-phenylenevinylene. *J. Phys. Chem. B* **2009**, *113*, 5083-5091.

17 Balamurugan, A.; Reddy, M. L. P.; **Jayakannan, M.** Carboxylic Functionalized Water Soluble π-Conjugated Polymer: Highly Selective and Efficient Chemosensor for Mercury (II) ions. *J. Polym. Sci. Polym. Chem.* **2009**, *47*, 5144-5157.

18 Resmi, R.; Amrutha, S. R.; **Jayakannan, M.** Control of Molecular Aggregation in Symmetrically Substituted ð-Conjugated Bulky Poly(p-phenylenevinylene) and their Copolymers. *J. Polym. Sci. Polym. Chem.* **2009**, *47*, 2631-2646.

19 Jinish Antony, M.; **Jayakannan, M.** Self-assembled Anionic Micellar Template for Polypyrrole, Polyaniline and Their Random Copolymer Nano-materials. *J. Polym. Sci. Polym. Phys.* **2009**, *47*, 830-846.

20 Anilkumar, P.; **Jayakannan, M.** Large-scale Synthesis of Polyaniline Nanofibers based on Renewable Resource Molecular Template. *J. Appl. Polym. Sci.* **2009**, *114*, 3531-3541.

21 Reddy J. S.; **Anand V. G.** Aromatic Expanded Isophlorins: Stable 30π Annulene Analogues with Diverse Structural Features. *J. Am. Chem. Soc*. **2009**, *131*, 15433.

22 Devi, G.; **Ganesh, K.N.;** 1, 4-linked 1, 2, 3-Triazole Des-peptidic Analogues of PNA (TzNA): Synthesis of TzNA Oligomers by "click" Reaction on Solid Phase and Stabilization of Derived Triplexes with DNA, Art DNA, *PNA:XNA*, **2010**, *1*, 68-75.

23 Sharma, N. K.; **Ganesh K. N.** Base dependent pyrrolidine ring pucker in aep-PNA monomers: NMR and PSEUROT analysis. *Tetrahedron*, **2010**, *66*, 9165-9170

24 Raman V.B.; **Ganesh K.N.** 8-Substituted Adeninyl Peptide Nucleic Acid (PNA): In-situ, On-resin Synthesis of 8-Br/NH2 Adeninyl PNA oligomers and their Complementation Studies with DNA. *Tetrahedron Lett*, **2010**, *51*, 6560-6564.

25 Sonar, M. V.; **Ganesh, K. N.** Switching Structures by H-bond Rearrangement: Transformation of β-structure in Poly-4S-Aminoproline to PPII Conformation. *Org. Lett.* **2010**, *12*, 5406-5409.

26 Mitra, R.; **Ganesh, K. N.** PNAs Grafted with (a/g, R/S)-aminomethylene Pendants: Regio- and Stereospecific Effects on DNA Binding and Improved Cell Uptake. *Chemical Communications*, **2010**, *12*, 5390-5393.

27 Patwa, A. N.; Gonnade, R. G.; Kumar, V. A.; Bhadbhade, M. M.; **Ganesh, K.N.** Ferrocene–bis (thymine/uracil) conjugates: Base Pairing Directed, Spacer Dependent Self Assembly and Supramolecular Packing. *J. Org. Chem.* **2010**, *75*, 8705-8708.

28 Mahima, G.; **Jayakannan, M.** Supramolecular Liquid Crystalline π-Conjugates: The Role of Aromatic π-stacking and van der Waals Forces on the Molecular Self-assembly of Oligo-Phenylenevinylenes. *J. Phys. Chem. B* **2010**, *114*, 12508- 12519. *(Appeared as cover page).*

29 Shekhar, S.; **Jayakannan, M.** Probing the Molecular Interactions at Conducting Polyaniline Nanomaterial Surface via a Pyrene Fluorophore. *J. Phys. Chem. C* **2010**, *114*, 15491-15498.

30 Jinish Antony, M.; **Jayakannan, M.** Molecular Template Approach for Evolution of Conducting Polymer Nanostructures: Tracing the Role of Morphology on Conductivity and Solid State Ordering. *J. Phys. Chem. B* **2010**, *114*, 1314-1324.

31 Anilkumar, P.; **Jayakannan, M.** A Novel Supramolecular Organogel Nanotubular Template Approach for Conducting Nanomaterials. *J. Phys. Chem. B* **2010**, *114*, 728-736.

32 Bandyopadhyay, A.; Agrawal, N.; Mali, S. M.; Jadhav, S. V.; **Gopi, H. N.** Tin(II) Chloride Assisted Synthesis of *N*-protected ã-amino â-keto Esters through Semipinacol Rearrangement, *Org. Biomol. Chem.* **2010**, *8*, 4855.

33 Kalle, A. M.; Mallika, A.; Badiger, J.; Alinakhi; **Talukdar, P.**; Sachchidanand, Inhibition of SIRT1 by a small Molecule Induces Apoptosis in Breast Cancer Cells. *Biochem. Biophys. Res.Commun.* **2010**, *401*, 13-19.

34 Pallavi, R.; Roy, N.; Nageshan, R. K.; **Talukdar, P.**; Pavithra, S. R.; Reddy, R.; Venketesh, S.; Kumar, R.; Gupta, A. K.; Singh, R. K.; Yadav, S. C.; Tatu, U. Heat Shock Protein 90 as a Drug Target Against Protozoan Infections: Biochemical Characterization of HSP90 from Plasmodium Falciparum and Trypanosoma Evansi and Evaluation of its Inhibitor as a Candidate drug. *J. Biol. Chem.* **2010**, *285*, 37964-37975.

35 Sengupta, A.; Khade, R. V.; **Hazra, P.** Solvation Dynamics of Coumarin 153 in SDS Dispersed Single Walled Carbon Nanotubes (SWNTs). *Chem. Phys. Lett.* **2010**, *501*, 33-38.

36 Sharma and. N. K.; **Ganesh, K. N.** Enhanced stability of G-Tetraplexes from Conformationally Constrained aep-PNA backbone. Org. Biomol. Chem. 2011, 9, 725-729.

37 Murthy, A. V. R.; Goel, M.; Patil, S.; **Jayakannan, M.** Probing the role of Chain length on the Diffusion Dynamics of π-conjugated Polymers by Fluorescence Correlation Spectroscopy. *J. Phys. Chem. B* **2011**, *115*, 10779-10788.

38 Balamurugan, A.; Reddy, M. L. P.; **Jayakannan, M.** Amphiphilic π-Conjugated Poly(m-Phenylene) Photosensitizer for Eu^{3+} ion: The role of Macromolecular Chain Aggregation on the Color Tunability of Lanthanides. *J. Phys. Chem. B* **2011**, *115*, 10789-10800.

39 Jinish Antony, M.; **Jayakannan, M.** Polyaniline Nano-scaffolds for Colorimetric Sensing of Biomolecules via Electron Transfer Process. Langmuir **2011**, *27*, 6268-6278.

40 Jinish Antony, M.; **Jayakannan, M.** Role of Anionic Micellar Template on the Morphology, Solid State ordering and Unusual Conductivity Trend in Poly(aniline-co-pyrrole) Nanomaterials. *J. Phys. Chem. B* **2011**, *115*, 6427-6436.

41 Bandyopadhyay, A.; **Gopi, H. N.** A Facile Transformation of Amino Acids to Functionalized Coumarins. *Org. Biomol. Chem.* **2011**, *9*, 8089.

42 Mali, S. M.; Bandyopadhyay, A.; Jadhav, S. V.; Kumar, M. G.; **Gopi, H. N.** Synthesis of α, β-unsaturated γ-amino Esters with Unprecedented high (*E*)-stereoselectivity and their Conformational Analysis in Peptides. *Org. Biomol. Chem.* **2011**, *9*, 6566.

43 Bandyopadhyay, A.; Mali, S.M.; Lunawat, P.; Raja, K. M.; **Gopi, H. N.** Synthesis and Structural Investigations of Functionalizable Hybrid β-hairpin. *Org. Lett.* **2011**, *13*, 4482.

44 Jadhav, S. V.; Bandyopadhyay, A.; Benke, S. N; Mali, S. M.; **Gopi, H. N.** A Facile Synthesis and Crystallographic Analysis of *N*-protected β-amino Alcohols and Short Peptaibols. *Org. Biomol. Chem.* **2011**, *9*, 4182.

45 Kishor, P.; **Jeganmohan, M.** Ruthenium-catalyzed Ortho-Alkenylation of Aromatic ketones with Alkenes by C-H Bond Activation. *Org. Lett.* **2011**, *13*, 6144.

46 Tanpure, A. A.; **Srivatsan, S. G.** A Microenvironment-sensitive Fluorescent Pyrimidine Ribonucleoside Analogue: Synthesis, Enzymatic Incorporation, and Fluorescence Detection of a DNA Abasic Site. *Chem. Eur. J.* **2011**, *17*, 12820-12827.

47 Pawar, M. G.; **Srivatsan, S. G.** Synthesis, Photophysical Characterization and Enzymatic Incorporation of a Microenvironment-sensitive Fluorescent Uridine Analog. *Org. Lett.* **2011**, *13*, 1114–1117.

48 **Srivatsan, S. G.;** Sawant, A. A. Fluorescent Ribonucleoside Analogues as Probes for Investigating RNA Structure and Function. *Pure Appl. Chem.* **2011**, *1*, 213-232.

49 Gupta, A.K.; Nicholls, J.; Debnath, S.; Rosbottom, I.; Steiner A.; **Boomishankar, R.** Organoamino Phosphonium Cations as Building Blocks for Hierarchical Supramolecular Assemblies. *Cryst. Growth Des.* **2011**, *11*, 555-564.

50 Gupta, A. K.; Kalita A.; **Boomishankar, R.** Synthesis and Supramolecular Structures of iso and Heteropolymetallates Assisted by Organoamino Phosphonium Cations. I*norg. Chim. Acta.* **2011**, *352*, 152-159 (Invited for a special issue celebrating the 70th birthday of Prof. S. S. Krishnamoorthy).

51 **Verma, S.;** Pravarthana, D. One-Pot Synthesis of Highly Monodispersed Ferrite Nanocrystals: Surface Characterization and Magnetic Properties, *Langmuir* **2011**, *27*, 13189-13197.

52 **Verma, S.;** Joy, P. A.; Kurian, S. Structural, Magnetic and Mossbauer Spectral Studies of Nanocrystalline $Ni_{0.5}Zn_{0.5}Fe_2O_4$ Ferrite Powders: An Effect of Elemental Stoichiometric Coefficients of Combustion Mixture. *J. Alloys Compounds* **2011**, 509, 8999-9004.

53 Kumar, S.; Kaul, I.; Biswas, P.; **Das, A.** Structure of 7-azaindole...2-fluoropyridine Dimer in a Supersonic Jet: Competition between N-H...N and N-H...F Interactions. *J. Phys. Chem. A* **2011**, *115*, 10299-10308.

54 Kumar, S.; Biswas, P.; Kaul, I.; **Das, A.** Competition Between Hydrogen-bonding and Dispersion Interactions in indole...pyridine dimer and $(indole)_2$...pyridine trimer Studied in a Supersonic Jet. *J. Phys. Chem. A* **2011**, *115*, 7461–7472.

55 Sengupta, A.; Khade, R. V.; **Hazra, P.** How Does the Urea Dynamics Differ from Water Dynamics inside the Reverse Micelle? *J. Phys. Chem. A* **2011**, *115*, 10398-10407.

56 Agarkar, S. A.; Kulkarni, R. R.; Dhas,V. V.; Chinchansure , A. A.; **Hazra, P.;** Joshi, S. P.; Ogale S.B. Isobutrin from Butea Monosperma (Flame of the Forest): A Promising New Natural Sensitizer Belonging to Chalcone Class. *ACS Appl. Mat. & Interfaces* **2011**, *3*, 2440-2444.

57 Sengupta, A.; Khade, R. V.; **Hazra, P.** pH Dependent Dynamic Behaviors of Flavin Adenine Dinucleotide (FAD) and FlavinMononucleotide (FMN) in Femtosecond to Nanosecond Time-scale. *J. Photochem. Photobiol. A: Chemistry* **2011**, *221, 105-112.*

58 Sunda A. P.; **Venkatnathan A.** Molecular Dynamics Simulations of Triflic acid and Triflate Ions/Water Mixtures: A Potential Electrolyte Component in Fuel Cells. *J. Comput. Chem.* **2011**, *32*, 3319-3328 **(appeared as cover).**

59 **Mukherjee, A.**, Entropy Balance in the Intercalation Process of an Anti-Cancer Drug Daunomycin. *J. Phys. Chem. Lett.* **2011,** *2* (24), 3021-3026.

60 Gourishankar, A.; **Ganesh, K. N.** (α, α-dimethyl)glycyl (dmg) PNAs: Achiral PNA Analogs that Form Stronger Hybrids with cDNA Relative to Isosequential RNA, Art DNA. *PNA:XNA*. **2012,** *3,* 1-9.

61 Umashankara, M.; Nanda, M.; Sonar, M.; **Ganesh, K. N.** 4(R/S)-Amino/Guanidino-Substituted Proline Peptides: Design, Synthesis and DNA Transfection Properties, *Chimia.* **2012,** *66,* 936–940.

62 Nanda M.; **Ganesh, K. N.;** 4(R/S)-Guanidinylprolyl Collagen Peptides: On-Resin Synthesis, Complexation with Plasmid DNA, and the Role of Peptides in Enhancement of Transfection. *J. Org. Chem*. **2012,** *77,* 4131 – 4135.

63 Mahima, G.; **Jayakannan, M.** Herringbone and Helical Self-assembly of π-conjugated Molecules in Solid State through CH/π Hydrogen Bond. *Chem. Eur. J.* **2012**, *18,* 11987-11993.

64 Mahima, G.; **Jayakannan, M.** CH/π Interaction Guided Molecular Self-assembly in π-conjugated Oligomers. *Chem. Eur. J.* **2012**, 18, 2867-2874.

65 Pramod, P. S.; Katamura, C.; Chapaker, S.; Balasubramaniam, N.; **Jayakannan, M.** Dextran Vesicular Carriers for Dual Encapsulation of Hydrophilic and Hydrophobic Molecules and Delivery into Cells. *Biomacromolecules* **2012**, *13*, *3627-3640.*

66 Anantharaj, S.; **Jayakannan, M.** Polymers from Amino acids: Development of Dual Ester-urethane Melt Condensation Approach and Mechanistic Aspects. *Biomacromolecules* **2012**, *13*, 2446- 2455.

67 Kashyap, S.; **Jayakannan, M.** Amphiphilic Diblocks Sorting into Multivesicular Bodies and Their Fluorophore Encapsulation Capabilities. *J. Phys. Chem. B* **2012**, *116*, 9820-9831.

68 Gopalsamy, S.; **Hotha, S.** $AuBr_3$ Mediated Glycosidations: Synthesis of Tetrasaccharide Motif of the Leishmania Donovani Lipophosphoglycan. *Glycoconj. J.* **2012**, *29*, 221-230.

69 Kayastha, A. K.; **Hotha, S.** Versatile Gold Catalyzed Transglycosidation at Ambient Temperature. *Chem. Commun.* **2012**, *48*, 7161-7163.

70 Vidadala, S. R.; Thadke, S. A.; **Hotha, S.;** Kashyap, S. Synthesis of Thioglycosides from Propargyl Glycosides Exploiting Alkynophilic Gold Catalyst. *J. Carb. Chem.* **2012,** *31,* 241-251.

71 Pati, D.; Shaikh, A. Y.; Das, S.; Nareddy, P. K.; Swamy, M. J.; **Hotha, S.;** Gupta, S. S. Controlled Synthesis of O-Glycopolypeptide Polymers and Their Molecular Recognition by Lectins. *Biomacromol.* **2012**, *13*, 1287-1295.

72 Mohite, A. R.; Sultane, P. R.; **Bhat, R. G.** $BF_3.Et_2O$ and Trifluoroacetic acid/Triethyl Amine Mediated Synthesis of Functionalized Piperidines. *Tetrahedron Lett.* **2012**, *53*, 30-35. (Highlighted in *ChemInform*, 2012, 43, Issue 17).

73 Mohite, A. R and **Bhat, R. G.** Enantiopure Synthesis of Side Chain-Modified α-Amino Acids and 5-*cis*-Alkylprolines. *J. Org. Chem.* **2012**, *77*, 5423–5428.

74 Sultane, P. R.; Mohite, A. R.; **Bhat, R. G.** Total synthesis of 1-deoxy-7,8a-di-*epi*-Castanospermine and Formal Synthesis of Pumiliotoxin-251D. *Tetrahedron Lett.* **2012**, *53*, 5856-5858.

75 Sultane, P. R.; **Bhat, R. G.** Stereoselective Approach to cis-2, 3-Disubstituted Piperidines via Reduction of N-Acyliminium Ion Intermediate: Enantioselective Synthesis of (+)-(2S, 3S)-CP-99,994 *J. Org. Chem.* **2012**, *77*, 11349-11354. (highlighted in Organic Chemistry Portal).

76 McFadden, K.; Fletcher, P.; Rossi, F.; Kantharaju, Umashankara, M.; Pirrone. V.; Rajagopal, S.; **Gopi, H. N.;** Krebs, F. C.; Martin-Garcia, J.; Shattock, R. J.; Chaiken, I. Antiviral Breadth and Combination Potential of Peptide Triazole HIV-1 Entry Inhibitors. *Antimicrob Agents Chemother*. **2012**, *56*, 1073.

77 Mali, S. M.; Schneider, T. F.; Bandyopadhyay, A.; Jadhav, S. J.; Werz, D. B.; **Gopi, H. N.** Thiazole-Carbonyl Interactions: A Case Study Using Phenylalanine Thiazole Cyclic Tripeptides. *Cryst. Growth Des.* **2012,** *12*, 5643.

78 Bandyopadhyay, A.; Jadhav, S. V.; **Gopi, H. N.** α/γ^4-Hybrid Peptide Helices: Synthesis, Crystal Conformations and Analogy with the α-helix. *Chem. Commun.* **2012,** *48*, 7170.

79 Mali, S. M.; Jadhav, S. V.; **Gopi, H. N.** Copper(II) Mediated Facile and Ultra fast Peptide Synthesis in Methanol. *Chem. Commun.* **2012**, *48*, 7085.

80 Bandyopadhyay, A.; **Gopi, H. N.** Hybrid Peptides: Direct Transformation of α/α, β-Unsaturated γ-Hybrid Peptides to α/γ-Hybrid Peptide 12-Helices. *Org. Lett*. **2012**, *14*, 2270.

81 Tanpure, A. A.; **Srivatsan, S. G.** Synthesis and Photophysical Characterization of a Fluorescent Nucleoside Analogue that Signals the Presence of an Abasic Site in RNA. *ChemBioChem.* **2012**, *13*, 2392–2399.

82 Rao, H.; Tanpure A. A.; Sawant, A. A.; **Srivatsan, S. G.** Enzymatic Incorporation of an Azide-modified UTP Analog into Oligoribonucleotides for Post-transcriptional Chemical Functionalization. *Nature Protocols* **2012,** *7*, 1097–1112**.**

83 Tanpure, A. A.; Patheja, P.; **Srivatsan, S. G.** Label-free Fluorescence Detection of the Depurination Activity of Ribosome Inactivating Protein Toxins. *Chem. Commun.* **2012,** *48*, 501–503. ***Selected as a Hot Article for ChemComm.***

84 Rao, H.; Sawant, A. A.; Tanpure A. A.; **Srivatsan, S. G.** Posttranscriptional Chemical Functionalization of Azide-modified Oligoribonucleotides by Bioorthogonal Click and Staudinger Reactions, *Chem. Commun.* **2012,** *48*, 498–500. ***Selected as a Hot Article for ChemComm and cover page article.***

85 Malwal, S. R.; Sriram, D.; Yogeeswari, P.; **Chakrapani, H.** Synthesis and Antimycobacterial Activity of Prodrugs of Sulfur Dioxide (SO_2) *Bioorg. Med. Chem. Lett.* **2012**, *22*, 3603-3606.

86 Dharmaraja, A. T.; Alvala, M.; Sriram, D.; Yogeeswari, P.; **Chakrapani, H.** Design, Synthesis and Evaluation of Small Molecule Reactive Oxygen Species Generators as Selective Mycobacterium Tuberculosis Inhibitors *Chem. Commun.* **2012**, *48*, 10325-10327.

87 Khodade, V. S.; Dharmaraja, A. T.; **Chakrapani, H.** Synthesis, Reactive Oxygen Species Generation and Copper-Mediated Nuclease Activity Profiles of 2-aryl-3-amino-1,4-Naphthoquinones *Bioorg. Med. Chem. Lett.* **2012**, *22*, 3766-3769.

88 Malwal, S. R.; Sriram, D.; Yogeeswari, P.; Konkimalla, V. B.; **Chakrapani, H.** Design, Synthesis and Evaluation of Thiol-Activated Sources of Sulfur Dioxide (SO_2) as Antimycobacterial Agents *J. Med. Chem.* **2012**, *55*, 553-557.

89 Dharamaraja, A. T.; Dash, T. K.; Konkimalla, V. B.; **Chakrapani, H.** Synthesis, Thiol-Mediated Reactive Oxygen Species Generation Profiles and Anti-Proliferative Activities of 2,3-Epoxy-1,4-Naphthoquinones *Med. Chem. Commun.* **2012,** 3, 219-224.

90 Deshmukh, S. C.; Roy, A.; **Talukdar, P.** Diastereoselective Construction of syn-α-Oxyamines via Three-component α-oxyaldehyde-dibenzylamine-alkyne Coupling Reaction: Application in the Synthesis of (+)-β-conhydrine and its Analogues. *Org. Biomol. Chem.* **2012,** *10*, 7536-7544.

91 Kand, D.; Mishra, P. K.; Saha, T.; Lahiri, M.; **Talukdar, P.** BODIPY Based Colorimetric Fluorescent Probe for Selective Thiophenol Detection: Theoretical and Experimental Studies. *Analyst* **2012,** *137*, 3921-3924.

92 Kand, D.; Kalle, A. M.; Varma, S. J.; **Talukdar, P.** A Chromenoquinoline-Based Fluorescent off-on Thiol Probe for Bioimaging. *Chem. Commun.* **2012,** *48*, 2722-2724.

93 Yadav, R.; **Kikkeri, R.** Carbohydrate Functionalized iron(III) Complexes as Biomimetic Siderophores, *Chem. Commun*. **2012**, 48, 1704-1706.

94 Yadav, R.; **Kikkeri, R.** Exploring the Effect of Sialic acid Orientation on Ligand-Recentor Interactions, *Chem. Commun*. **2012**, 48, 7265-2767.

95 Kishor, P.; **Jeganmohan, M.** Highly Regio-and Stereoselective Ruthenium(II)-Catalyzed Direct ortho-Alkenylation of Aromatic and Heteroaromatic Aldehydes with Activated Alkenes under Open Atmosphere. *Org. Lett.* **2012,** *14*, 1134 (Highlited in Synfacts **2012,** 8, 553).

96 Ravi Kiran, CG.; **Jeganmohan, M.** Ruthenium-Catalyzed Regioselective Cyclization of Aromatic Ketones with Alkynes: An Efficient Route to Indenols and Benzofulvenes. *Eur. J. Org. Chem.* **2012,** 417.

97 Ravi Kiran, CG.; **Jeganmohan, M.** Regioselective Synthesis of Isocoumarins by Ruthenium-Catalyzed Aerobic Oxidative Cyclization of Aromatic Acids with Alkynes. *Chem. Commun.* **2012,** *48*, 2030.

98 Ravi Kiran CG.; Pimparkar, S.; **Jeganmohan, M.** Ruthenium-Catalyzed Highly Regioselective Cyclization of Ketoximes with Alkynes by C-H Bond Activation: A Practical Route to Isoquinolines Synthesis. *Org. Lett.* **2012,** *14*, 3032.

99 Kishor, P.; Pimparkar, S.; Padmaja, M.; **Jeganmohan, M.** Ruthenium-catalyzed Regioselective Oxidative Coupling of Aromatic and Heteroaromatic Esters with Alkenes under Open Atmosphere. *Chem Commun.* **2012,** *48*, 2030.

100 Ravi Kiran, CG.; **Jeganmohan, M.** Regioselective *Ortho*-Arylation and Alkenylation of *N-Alkyl* Benzamides with Boronic Acids via Ruthenium-Catalyzed C-H Bond Activation: An Easy Route to Fluorenones Synthesis. *Org. Lett.* **2012,** *14*, 5246 (Highlited in *Synfacts* **2013,** 9, 0091).

101 Chaudhari, A. K.; Joarder, B.; Riviere, E.; Rogez, G.; **Ghosh, S. K.** Nitrate Bridged Pseudo Double Propeller Type Lanthanide (III)-Copper (II) Heterometallic Clusters: Syntheses, Structures, and Magnetic Properties. *Inorg. Chem.* **2012**, *51*, 9159–9161. (Highlighted in Cheminform).

102 Nagarkar, S. S.; Das, R.; Poddar, P.; **Ghosh, S. K.** A Bistable Dynamic Coordination Polymer Showing Reversible Structural and Functional Transformations *Inorg. Chem.* **2012**, *51*, 8317-8321.

103 Joarder, B.; Chaudhari, A. K.; Rogez, G.; **Ghosh, S. K.** A Carboxylate Based Dinuclear Dysprosium (III) Cluster Exhibiting Slow Magnetic Relaxation Behavior *Dalton Trans.* **2012**, *41*, 7695-7699.(One of the Top ten most accessed Dalton Trans. articles in May 2012).

104 Nagarkar, S. S.; Chaudhari, A. K.; **Ghosh, S. K.** Role of Temperature on Framework Dimensionality: Supramolecular Isomers of $Zn_3(RCOO)_8$ Based Metal Organic Frameworks *Cryst. Growth Des.* **2012**, *12*, 572-576.

105) Joarder, B.; Chaudhari, A. K.; **Ghosh, S. K.** A Homochiral Luminescent 2D Porous Coordination Polymer with Collagen-Type Triple Helices Showing Selective Guest Inclusion *Inorg. Chem.* **2012**, *51*, 4644-4649.

106 Nagarkar, S. S.; Chaudhari, A. K.; **Ghosh, S. K.** Selective CO_2 Adsorption in a Robust and Water-Stable Porous Coordination Polymer with New Network Topology *Inorg. Chem.* **2012**, *51*, 572-576.

107 **Ghosh, S. K.**; Kitagawa, S. Surface Pore Engineering of Porous Coordination Polymers in *Metal-Organic Frameworks: Design and Application* (Eds.: MacGillivray L. R.) *Wiley*, **2010**, 165-192. (Book chapter).

108 Gupta, A. K.; Chipem F. A. S.; **Boomishankar, R.** A 2-pyridyl (py) Attached Phosphine Imine $[P(Npy)(NHpy)_3]$ and an Imido Phosphinate ion $[P(Npy)_2(NHpy)_2]^-$ in its Ag(I) Complex. *Dalton Trans.* **2012,** *41,* 1848-1853.

109 Gupta, A. K.; Steiner A.; **Boomishankar, R.** Tri-, Hepta- and Octa-nuclear Ag(I) Complexes Derived from 2-pyridyl Functionalized Tris(amido)phosphate Ligand. *Dalton Trans.* **2012,** *41*, 9753-9759.

110 Kale, S. N.; Jadhav, A. D.; **Verma, S.**; Koppikar, S. J.; Kaul-Ghanekar, R. S.; Dhole, D.; Ogale, S. B. Characterization of Biocompatible $NiCo_2O_4$ Nanoparticles for Applications in Hyperthermia and Drug Delivery. *Nanomedicine, Nanotechnology, Biology and Medicine* **2012**, *8*, 452-459.

111 Phadatare, S. D.; Sharma K. K. K.; **Rao, B. S. M.;** Naumov, S.; Sharma, G. K. Spectral characterization of guanine C4-OH adduct: A Radiation and Quantum Chemical Study**.** *J. Phys. Chem. B* **2011,** *115*, 13650–13658.

112 Karnawat, V.; Jayanth, N.; **Puranik, M.** Substrate Recognition in Multisubstrate Nucleic Acid Enzymes, *Curr Sci*. **2012**, *102,* 298-313.

113 Kumar, S.; Mukherjee, A.; **Das, A.** Structure of indole...imidazole Heterodimer in a Supersonic Jet: A gas phase study on the Interaction between the Aromatic side chains of Tryptophan and Histidine residues in Proteins. *J. Phys. Chem. A* **2012,** *116,* 11573-11580.

114 Kumar, S.; **Das, A.** Effect of Acceptor Heteroatoms on π-hydrogen Bonding Interactions: A study of indole…thiophene Heterodimer in a Supersonic Jet. *J. Chem. Phys.* **2012,** *137,* 094309.

115 Kumar, S.; **Das, A.**Mimicking Trimeric Interactions in the Aromatic side chains of the Proteins: A gas phase study of indole...$(pyrrole)_2$ heterotrimer. *J. Chem. Phys.* **2012,** *136,* 174302. (Selected for Virtual Journal of Biological Physics Research, Vol. 23, May 15, 2012, Section: Protein Conformational Dynamics/Folding)

116 Kumar, S.; Pande, V.; **Das, A.** π-hydrogen Bonding wins over Conventional Hydrogen Bonding Interaction: A Jet-cooled Study of indole...furan Heterodimer. *J. Phys. Chem. A* **2012,** *116,* 1368-1374.

117 Sengupta, A.; Sasikala, W. D.; **Mukherjee, A.; Hazra, P.** Comparative Study of Flavins Binding with Human Serum Albumin: a Fluorometric, Thermodynamic, and Molecular Dynamics Approach. *ChemPhysChem*. **2012**, *13*, 2142-2153.

118 Ramya K. R.; Kumar G. V. P.; **Venkatnathan A.** Raman spectra of Vibrational and Librational modes of Methane Clathrate Hydrates using Density Functional Theory, *J. Chem. Phys.* **2012**, *136,* 174305-5.

119 Pahari S.; Choudhary S.; Pandey P. R.; More M.; **Venkatnathan A.;** Roy S. Molecular Dynamics Simulation of Phosphoric Acid Doped Monomer of Polybenzimidazole: A Potential Component Polymer Electrolyte Membrane of Fuel Cell, *J. Phys. Chem. B* **2012**, *116*, 7357-7366.

120 Ramya K. R.; **Venkatnathan A.** Stability and Reactivity of Methane Clathrate Hydrates: Insights from Density Functional Theory, *J. Phys. Chem. A* **2012**, *116*, 7742-45.

121 Mane M.; **Venkatnathan A.;** Ghatak K.; Vanka K. Exploring the Potential of Doped Zero-Dimensional Cages for Proton Transfer in Fuel Cells: A Computational Study, *J. Phys. Chem. B* **2012**, *116*, 9803-9811.

122 Sunda A. P.; **Venkatnathan A.** Atomistic Simulations of Structure and Dynamics of Hydrated Aciplex Polymer Electrolyte Membrane, *Soft Matter* **2012**, *8*, 10827-10836.

123 Sasikala, W. D.; **Mukherjee, A.** Molecular Mechanism of Direct Proflavine-DNA Intercalation: Evidence for Drug-Induced Minimum Base-Stacking Penalty Pathway. *J. Phys. Chem. B* **2012**, *116* (40), 12208-12212.

124 Wilhelm, M.; **Mukherjee, A.;** Bouvier, B.; Zakrzewska, K.; Hynes, J. T.; Lavery, R. Multistep Drug Intercalation: Molecular Dynamics and Free Energy Studies of the Binding of Daunomycin to DNA. *J. Am. Chem. Soc.* **2012**, *134* (20), 8588-8596.

125 Borghetti, P; **Ghosh, P.;** Castellarin-Cudia, C.; Goldoni, A.; Floreano, L.; Cossaro, A. ;Verdini, A.; Gebauer, R.; Drera, G.; Sangaletti, L. Functional K-doping of Eumelanin Thin Films: DFT Theory and Soft X-ray Spectroscopy Experiments in the Frame of the Macrocyclic Protomolecule Model. *J. Chem. Phys*. **2012**, *136*, 204703.

126 Santra, S.; Ranjan, P.; Bera, P.; **Ghosh, P.;** Mandal, S. K. Anchored Palladium Nanoparticles onto Single Walled Carbon Nanotubes: Efficient Recyclable Catalyst to N-Containing Heterocycles. *RSC Advances* **2012**, *2*, 7523 - 7533.

127 Kaul, I.; Joshi, N.; **Ballav N.; Ghosh, P.** Hydrogenation of Ferrimagnetic Graphene on a Co Surface: Significant Enhancement of Spin Moments by C-H Functionality. *J. Phys. Chem. Lett.* **2012,** *3*, 2582-2587.

128 Joshi, N.; **Ballav, N.; Ghosh, P.** Hydrogen-induced Reversal of Spin Alignment in Graphene Supported on Ni(111) Surface. *Phys. Rev. B* **2012,** *86*, 121411(R).

129 **Ganesh K. N.;** Krishnan, Y. Nucleic Acids – Chemistry and Applications. *J. Org. Chem.* **2013,** *78*, 12283-12287.

130 Surnar B.; **Jayakannan, M.** Stimuli-responsive Polycaprolactone Vesicles for Dual Drug Delivery under GI Tract, *Biomacromolecules* **2013**, *14*, 4377-4387.

131 Singh, H.; Balamurugan, A.; **Jayakannan, M.** Solid State Assemblies and Photophysical Characteristics of Linear and Bent-core π-Conjugated Oligophenylenevinylenes. *ACS Appl. Mater. Interfaces* **2013**, *5*, 5578 – 5591.

132 Balamurugan A.; Reddy, M. L. P.; **Jayakannan, M.** π-conjugated Polymer-Eu^{3+} Complexes: A Versatile Luminescent Molecular probe for Temperature Sensing. *J. Mater. Chem. A* **2013**, *1*, 2256-2266.

133 Uma Sridhar; Pramod, P. S.; **Jayakannan, M.** Creation of Dextrin Vesicles and Their Loading-Delivering Capabilities. *RSC Advances* **2013,** *3*, 21237-21241.

134 Shinde, S. D.; **Jayakannan, M.** New Amphiphilic Sulfonic Acid Dopant-Cum-Template for Diverse Conducting Polyaniline Nanomaterials, *J. Apply. Polym. Sci*. **2013**, *127*, 1781- 1793.

135 Kayastha, A. K.; **Hotha, S.** Gold-catalyzed Glycosidation for the Synthesis of Trisaccharides by applying the Armed-disarmed Strategy. *Beil. J. Org. Chem.* **2013**, *9*, 2147-2155.

136 Thadke, S. A.; Mishra, B.; **Hotha, S.** Facile Synthesis of beta- and alpha-Arabinofuranosides and Application to Cell Wall Motifs of M. tuberculosis. *Org. Lett.* **2013**, *15*, 2466-2469.

137 Dhaware, V.; Shaikh, A. Y.; Kar, M.; **Hotha, S.;** Gupta, S. S. Synthesis and Self-assembly of Amphiphilic Homoglycopolypeptide. *Langmuir* **2013**, *29*, 5659-5667.

138 Rao, B. V.; Dhokale, S.; Rajamohanan, P. R.; **Hotha, S.** A Tetrazine Templated Method for the Synthesis of Ternary Conjugates. *Chem. Commun.* **2013**, *49*, 10808-10810.

139 **Bhat, R. G.;** Mohite, A. R. Synthesis of α, β-Unsaturated Carboxylic Acids and Esters Provisional Patent Filed in India, App No.: 2437/MUM/2013.

140 Navale, B. S.; **Bhat, R. G.** Copper(I) iodide-DMAP Catalyzed Homo-and Heterocoupling of Terminal Alkynes. *RSC Advances* **2013**, *3*, 5220-5226.

141 Mohite, A. R.; **Bhat, R. G.** A Practical and Convenient Protocol for the Synthesis of (E)-α, β-Unsaturated Acids *Org. Lett.* **2013**, *15*, 4564-4567. *(highlighted in Organic Chemistry Portal)

142 Jadhav, S. V.; Singh, S. K.; Reja, R. M; **Gopi, H. N.** γ-Amino acid Mutated α-coiled Coils as Mild Thermal Triggers for Liposome Delivery. *Chem Commun*. **2013,** 49**, 11065.**

143 Shankar, S. S.; Benke, S. N.; Nagendra, N.; Srivastava, P. L.; Thulasiram, H.V.; **Gopi, H. N.** Self-assembly to Function: Design, Synthesis, and Broad Spectrum Antimicrobial Properties of Short hybrid *E*-vinylogous Lipopeptides. *J. Med. Chem*. **2013**, *56*, 8468.

144 Jadhav, S. V.; Misra, R.; Singh, S. K.; **Gopi, H. N.** Efficient Access to Enantiopure γ^4-Residues with Proteinogenic side chains and Structural Investigation of γ^4-Asn and γ^4-Ser in Hybrid Peptide Helices. *Chem. Eur. J.* **2013**, *19*, 5955.

145 Jadhav, S.V.; **Gopi, H. N.** Remarkable Thermoresponsive Nanofibers from γ-Peptides. *Chem. Commun*. **2013,** *49,* 9179.

146 Mali, S. M.; Bhaisare, R. D; **Gopi, H. N.** Thioacids Mediated Selective and Mild *N*-Acylation of Amines. *J. Org. Chem*. **2013**, *78*, 5550.

147 Sonti, R.; **Gopi, H. N.;** Muddegowda, U.; Ragothama, S.; Balaram, P. A Designed Three-stranded β-sheet in an α/β Hybrid Peptide. *Chem. Eur. J*. **2013**, *19*, 5955.

148 Jadhav, S. V.; Bandyopadhyay, A.; **Gopi, H. N.** Protein Secondary Structure Mimetics: Crystal Conformations of α/γ^4-Hybrid Peptide12-Helices with Proteinogenic side chains and their Analogy with á- and â-peptide Helices. *Org. Biomol. Chem*. **2013**, *11*, 509.

149 Ganesh Kumar, M.; Mali, S. M.; **Gopi, H. N.** Synthesis and Stereochemical Analysis of β-nitromethane Substituted γ-amino acids and Peptides. *Org. Biomol. Chem*. **2013**, *11*, 803.

150 Pawar, M. G.; **Srivatsan, S. G.** Environment-responsive Fluorescent Nucleoside Analogue Probe for Studying Oligonucleotide Dynamics in a Model Cell-like Compartment. *J. Phys. Chem. B* **2013**, *117*, 14273-14282.

151 Pawar, M. G.; Nuthanakanti, A.; **Srivatsan, S. G.** Heavy Atom Containing Fluorescent Ribonucleoside Analog Probe for the Fluorescence Detection of RNA-ligand Binding. *Bioconjugate Chem*. **2013**, *24*, 1367-1377.

152 Peters, J. P.; Yelgaonkar, S. P.; **Srivatsan, S. G.**; Tor, Y.; Maher III, L. J. Mechanical Properties of DNA-like Polymers. *Nucl. Acid. Res*. **2013**, *41*, 10593-10604.

153 Tanpure, A. A.; Pawar, M. G.; **Srivatsan, S. G.** Fluorescent Nucleoside Analogs: Probes for Investigating Nucleic Acid Structure and Function. *Isr. J. Chem*. **2013**, *53*, 366-378.

154 Sabale, P. M.; Nuthanakanti, A.; **Srivatsan, S. G.** Synthesis and Fluorescence Properties of a full set of Extended RNA Base Analogues. *Ind. J. Chem*. **2013**, *52A*, 1004-1013.

155 Sharma, K.; Sengupta, K.; **Chakrapani, H.** Nitroreductase Activated Nitric Oxide Prodrugs *Bioorg. Med. Chem. Lett.* **2013**, *23*, 5964–5967.

156 Sharma, K.; Iyer, I.; Sengupta, K.; **Chakrapani, H.** INDQ NO, a Bioreductively Activated Nitric Oxide Prodrug *Org. Lett.* **2013**, *15*, 2636-2639.

157 Malwal, S. R.; Gudem, M.; **Hazra, A.; Chakrapani, H.** Benzosultines as Sulfur Dioxide (SO_2) Donors *Org. Lett.* **2013**, *15*, 1116-1119.

158 Saha, T.; Kand, D.; **Talukdar, P.** A Colorimetric and Fluorometric BODIPY Probe for Rapid, Selective Detection of H_2S and its Application in Live cell Imaging. *Org. Biomol. Chem.* **2013,** *11*, 8166-8170.

159 Gening, M. L.; Tsvetkov, Y. E.; Titov, D. V.; Gerbst, A. G.; Yudina, O. N.; Grachev, A. A.; Shashkov, A. S.; Vidal, S.; Imberty, A.; Saha, T.; Kand, D.; **Talukdar, P.**; Pier, G. B.; Nifantiev, N. E., Linear and Cyclic oligo-β-(1 → 6)-D-glucosamines: Synthesis, Conformations, and Applications for Design of a Vaccine and Oligodentate Glycoconjugates. *Pure Appl. Chem.* **2013,** *85*, 1879-1891.

160 Kand, D.; Chauhan, D. P.; Lahiri, M.; **Talukdar, P.** δ-Unsaturated γ-amino acids: Enantiodivergent Synthesis and cell Imaging Studies. *Chem. Commun.* **2013,** *49*, 3591-3593.

161 Kand, D.; Kalle, A. M.; **Talukdar, P.** Chromenoquinoline-based Thiol Probes: A Study on the Quencher Position for Controlling Fluorescent off-on Characteristics. *Org. Biomol. Chem.* **2013,** *11*, 1691-1701.

162 Bavireddi, H.; **Kikkeri, R.** Glyco-β-cyclodextrin Capped Quantum Dots: Synthesis, Cytotoxicity and Optical Detection of Carbohydrate-protein Interactions, *Analyst* **2012**, 137, 5123-7.

163 **Kikkeri, R.;** Padler-karavani, V.; Diaz, S.; Verhagen, A.; Yu, H.; Cao, H. Langereis, M. A.; De Groot, R. J.; Chen, X.; Varki, A. Quantum dot Nanometal Surface Energy Transfer Based Biosensing of Sialic Acid Compositions and Linkages in Biological Samples. *Anal. Chem*. **2013**, *85*, 3864-70.

164 Bavireddi, H.; Bharate, P.; **Kikkeri, R.** Probing Carbohydrate-Carbohydrate Interactions by Photoswitchable Supramolecular Glycoclutures. *Chem. Commun*. **2013**, *49*, 3988-90.

165 Azzouz, N.; Kamena, F.; Laurino, P.; **Kikkeri, R.**; Mercier, C.; Cesbron-Delauw, M. F.; Dubremetz, J. F.; De Cola, L.; Seeberger, P. H.; Toxoplasma Gondii Secretory Proteins Bind to Sulphated Heparin Structures, *Glycobiology* **2013**, *23*, 106-20.

166 Bavireddi, H.; Bharate, P.; **Kikkeri, R.** Use of Boolean and Fuzzy Logics in Lactose Glycocluster Research, *Chem. Commun*. **2013**, 49, 9185-7.

167 Reddy, M. C.; **Jeganmohan, M.** Ruthenium-Catalyzed Highly Regio- and Stereoselective Hydroarylation of Aryl Carbamates with Alkynes via C-H Bond Activation. *Chem Commun.* **2013,** *49,* 481.

168 Reddy, M. C.; **Jeganmohan, M.** Ruthenium-Catalyzed Selective Aerobic Oxidative ortho-Alkenylation of Substituted Phenols with Alkenes through C-H Bond Activation. *Eur. J. Org. Chem.* **2013,** 1150.

169 Ravi Kiran CG, Pimparkar, S.; **Jeganmohan, M.** Ruthenium-catalyzed Intramolecular Selective Halogenation of O-methylbenzohydroximoyl Halides: A New Route to Halogenated Aromatic Nitriles. *Chem Commun.* **2013,** *49,* 3146.

170 Ravi Kiran CG, Pimparkar, S.; **Jeganmohan, M.** A Regioselective Synthesis of 1 Haloisoquinolines via Ruthenium-catalyzed Cyclization of O-methylbenzohydroximoyl Halides with Alkynes. *Chem. Commun.* **2013,** *49,* 3703.

171 Reddy, M. C.; Manikandan, R.; **Jeganmohan, M.** Ruthenium-catalyzed Aerobic Oxidative Cyclization of Aromatic and Heteroaromatic Nitriles with Alkynes: A New Route to Isoquinolones. *Chem. Commun.* **2013,** *49,* 6060.

172 Kishor P; **Jeganmohan, M.** Ruthenium-catalyzed Oxidative *ortho*-benzoxylation of Acetanilides with Aromatic Acids. *Chem. Commun.* **2013,** *49,* 9651.

173 Patil, S.; Patil, S.; Gawali, S.; Shende, S.; Jadhav, S.; **Basu, S.** Novel Self-Assembled Lithocholic Acid Nanoparticles for Drug Delivery in Cancer. *RSC Adv.* **2013**, *3*, 19760-19764.

174 Patil, S.; Gawali, S.; Patil, S.; **Basu, S.** Synthesis, Characterization and in Vitro Evaluation of Novel Vitamin D3 Nanoparticles as Versatile Platform for Drug Delivery in Cancer. *J. Mater. Chem. B* **2013,** *1*, 5742-5750.

175 Gadekar S. C.; Reddy B. K.; **Anand V. G.** Metal Assisted Cyclomerization of N-Confused Dipyrrins into Expanded Norroles. *Angew. Chem. Int. Ed*. **2013**, *52*, 7164.

176 Gopalakrishna T. Y.; Reddy J. S.; **Anand V. G.** Antiaromatic Supramolecules: F···S, F···Se, and F···π Intermolecular Interactions in 32π Expanded Isophlorins. *Angew. Chem. Int. Ed*. **2013**, *52*, 1763.

177 Chaudhari, A. K.; Nagarkar, S. S.; Joarder, B.; Mukherjee, S.; **Ghosh, S. K.** Structural Dynamism and Controlled Chemical Blocking/Unblocking of Active Coordination Space of a Soft Porous Crystal. *Inorg. Chem.* 2013, *52*, 12784-12789.

178 Nagarkar, S. S.; Joarder, B.; Chaudhari, A. K.; Mukherjee, S.; **Ghosh, S. K.** Highly Selective Detection of Nitro-Explosive by a Luminescent Metal-Organic Framework. *Angew. Chem. Int. Ed.* **2013**, *52*, 2881-2885.

179 Joarder, B.; Chaudhari, A. K.; Nagarkar, S. S.; Manna, B.; **Ghosh, S. K.** Amino Acid Based Dynamic Metal-Biomolecule Framework *Chem. Eur. J.* **2013**, *19*, 11178-1183.

180 Chaudhari, A. K.; Nagarkar, S. S.; Joarder, B.; **Ghosh, S. K.** A Continuous π-Stacked Starfish Array of Two-Dimensional Luminescent MOF for Detection of Nitro Explosives. *Cryst. Growth Des*. **2013**, *13*, 3716-3721.

181 Chaudhari, A. K.; Mukherjee, S.; Nagarkar, S. S.; Joarder, B.; **Ghosh, S. K.** Bi-porous Metal-Organic Framework With Hydrophilic and Hydrophobic Channels: Selective Gas Sorption and Reversible Iodine Uptake Studies. *CrystEngComm.* **2013**, *14*, 9465-9471.

182 Mukherjee, S.; Chaudhari, A. K.; Xue, S.; Tang, J.; **Ghosh, S. K.** An Asymmetrically Connected Hexanuclear Dy^{III}_6 Cluster Exhibiting Slow Magnetic Relaxation. *Inorganic Chemistry Communications* **2013**, *35*, 144-148.

183 Manna, B.; Chaudhari, A. K.; Joarder, B.; Karmakar, A.; **Ghosh, S. K.** Dynamic Structural Behavior and Anion-Responsive Tunable Luminescence of a Flexible Cationic Metal-Organic Framework. *Angew. Chem. Int. Ed*. **2013**, *52*, 998-1002. (Highlighted: Advances in Engineering)

184 Gupta, A. K.; Reddy S. A. D.; **Boomishankar, R.** Facile Formation of Stable Tris(imido)phosphate Trianions as its tri- and Hexa-nuclear Pd(II) Complexes in Polar Solvents. *Inorg. Chem.* **2013,** *52,* 7608-7614.

185 Gupta, A. K.; Nagarkar S. S.; **Boomishankar, R.** Zn(II) Coordination Polymer of an in-situ Generated 4-pyridyl (^{4}Py) Attached bis(amido)phosphate Ligand, $[PO_2(NH^4Py)_2]^-$ Showing Preferential Water Uptake over Aliphatic Alcohols. *Dalton Trans.* **2013,** *42,* 10964-10970.

186 Balamurugan, A.; Gupta, A. K.; **Boomishankar, R.;** Reddy M. L.; **Jayakannan, M.** Heavy Atom Effect Driven Organic Phosphors and Their Luminescent Lanthanide Metal–Organic Frameworks. *Chem Plus Chem* **2013,** *78,* 737-745.

187 Dhara, B.; **Ballav, N.,** In Situ Generation of Conducting Polymer in a Redox-Active Metal–Organic Gel. *RSC Advances* **2013**, *3*, 4909-4913.

188 Rajendra, R.; **Ballav, N.** Discriminative Response of Aliphatic and Aromatic Dithiol in the Self-Assembly of Gold Nanoparticles. *RSC Advances* **2013**, *3*, 15622-15625.

189 Thampi, A.; Babu K.; **Verma S.** Large Scale Solvothermal Synthesis and a Strategy to Obtain Stable Langmuir–Blodgett Film of $CoFe_2O_4$ Nanoparticles. *Journal of Alloys and Compounds* **2013**, *564,* 143-150.

190 Milan-Garces, E. A.; Kaptan, S.; **Puranik, M.** Mode-specific Reoganization energies and Ultrafast Solvation Dynamics of Tryptophan from Raman Line-Shape Analysis. *Biophys. J.* **2013**, *105,* 211-221.

191 Kumar, S.; **Das, A.** Observation of Exclusively π-stacked Heterodimer of Indole and Hexafluorobenzene in the Gas Phase. *J. Chem. Phys.* **2013,** *139,* 104311.

192 Gavvala, K.; Sengupta, A.; Koninti, R. K.; **Hazra, P.** Prototropical and Photophysical Properties of an Anti Cancer Drug, Ellipticine Inside the Nano-Cavities of Molecular Containers. *J. Phys. Chem. B* **2013**, *117*, 14099-14107.

193 Sengupta, A.; Gavvala, K.; Koninti, R. K.; Chaudhuri, H.; **Hazra, P.** Folding Dynamics of Flavin Adenine Dinucleotide (FAD) inside Non-aqueous and Aqueous Reverse Micelles. *Chem. Phys. Lett.* **2013**, *584*, 76-73.

194 Topotecan. Gavvala, K.; Sengupta, A.; Koninti, R. K.; **Hazra, P.** Supramolecular Host Inhibited Excited State Proton Transfer and Fluorescence Switch of an Anti-cancer Drug, *ChemPhysChem.* **2013**, *14*, 3375-3383.

195 Gavvala, K.; Sengupta, A.; **Hazra, P.** Modulation of Photophysics and pKa Shift of an Anticancer Drug, Camptothecin, in the Nanocavities of Supramolecular Hosts. *Chem Phys Chem.* **2013**, *14*, 532-542.

196 Gavvala, K.; Sasikala, W. D.; Sengupta, A.; Dalvi, S. A.; **Mukherjee, A.; Hazra, P.** Modulation of Excimer Formation of 9-(dicyano-vinyl) julolidine by the Macrocyclic Hosts. *Phys. Chem. Chem. Phys.* **2013**, *15*, 330-340.

197 Kadlag, K. P.; Rao, M. J.; **Nag, A.** *Ligand-Free, Colloidal, and Luminescent Metal Sulfide Nanocrystals. J. Phys. Chem. Lett.* **2013**, *4*, 1676-1681.

198 M. More, S. Pahari, Roy S.; **Venkatnathan A.** Characterization of Structure and Dynamics of Phosphoric Acid Doped Benzimidazole Mixtures: A Molecular Dynamics Study, *J. Mol. Mod.* **2013**, *19*, 109-118.

199 Sunda A. P.; **Venkatnathan A.** Molecular Dynamics Simulations of Side Chain Pendant of Perfluorosulfonic Acid Polymer Electrolyte Membranes, *J. Mater. Chem. A*. **2013,** *1*, 557-569.

200 Sunda A. P.; More M.; **Venkatnathan A.** A Molecular Investigation of Nanostructure and Dynamics of Phosphoric/Triflic Acid Blends of Hydrated ABPBI [poly(2,5-benzimidazole)] Polymer Electrolyte Membrane. *Soft Matter* **2013**, *9*, 1122-1132.

201 Sunda A. P.; **Venkatnathan A.** Parametric Dependence on Shear Viscosity of SPC/E Water from Equilibrium and Non-equilbrium Molecular Dynamics Simulations. *Molecular Simulation* **2013**, *39*, 728-733.

202 Ramya K. R.; **Venkatnathan A.** Vibrational Raman Spectra of Hydrogen Clathrate Hydrates from Density Functional Theory. *J. Chem. Phys.* **2013**, *138*, 124305-6.

203 Ramya K. R.; **Venkatnathan A.** Density Functional Theory Study of Oxygen Clathrate Hydrates, *Indian J Che, Sec A*, special issue on Complex Chemical Systems, **2013**, *52A*, 1061-1065.

204 Ramya K. R.; **Venkatnathan A.** Characterization of Interaction Energy and Vibrational Raman Spectra of Nitrogen Clathrate Hydrates. *Comp. Theo. Chem.* **2013**, *1024*, 1-4.

205 Kumar M.; **Venkatnathan A.** Mechanism of Proton Transport in Ionic Liquid Doped Perfluorosulfonic Acid Membranes. *J. Phys. Chem. B* **2013**, *117*, 14449-14456.

206 Kulkarni, M.; **Mukherjee, A.** Sequence Dependent Free Energy Profiles of localized B- to A-form Transition of DNA in water. *J. Chem. Phys.* **2013**, *139* (15).

207 **Mukherjee, A.**; Sasikala, W. D. Drug-DNA Intercalation: From Discovery to the Molecular Mechanism. *Dynamics of Proteins and Nucleic Acids* **2013**, *92*, 1-62.

208 Sasikala, W. D.; **Mukherjee, A.** Intercalation and de-intercalation Pathway of Proflavine Through the Minor and Major Grooves of DNA: Roles of Water and Entropy. *Phys. Chem. Chem. Phys.* **2013**, *15* (17), 6446-6455.

209 Joshi, N.; **Ghosh, P.** Substrate Induced Changes in the Magnetic and Electronic Properties of Hexagonal Boron Nitride. *Phys. Rev. B* **2013,** 87, 235440.

210 **Ghosh, P.**; Camellone, M. F.; Fabris, S. Fluxionality of Au Clusters at Ceria Surfaces During CO oxidation: Relationships among Reactivity, Size, Cohesion, and Surface Defects from DFT Simulations. *J. Phys. Chem. Lett.* **2013,** 4, 2256-2263.

211 Santra, S.; Hota, P. K.; Bhattacharyya, R.; Bera,P.; **Ghosh, P.;** Mandal, S. K. Palladium Nanoparticles on Graphite Oxide: A Recyclable Catalyst for the Synthesis of Biaryl Cores. *ACS Catalysis.* **2013,** *3*, 2776-2789.

212 Jain, D. R.; Libi, A. V.;Lahiri, M.; **Ganesh, K.N.**; Influence of Pendant Chiral Cγ-(alkylideneamino/guanidino)Cationic Sidechains of PNA Backbone on Hybridization with Complementary DNA/RNA and Cell Permeability. *J. Org. Chem.***2014,** *79*, 9567-9577.

213 Jain, D. R.; **Ganesh, K. N.**; Clickable CγAzido(methylene/butylene) Peptide Nucleic Acids and Their Clicked Fluorescent Derivatives: Synthesis, DNA Hybridization Properties, and Cell Penetration Studies. *J. Org. Chem.* **2014,** *79*, 6708 – 6714.

214 Karnati, N.; **Jayakannan, M.** π-Conjugated Polymer Anisotroipic Organogel Nano-fibrous Assemblies for Thermo-responsive Photonic Switches. *ACS Appl. Mater. Interfaces*. **2014**, DOI 10.1021/am505479z

215 Pramod, P. S.; Shah, R.; Sonali, C.; Balasubramanian, N.; **Jayakannan, M.** Polysaccharide Nano-vesicular Multidrug Carrier for Synergistic Killing of Cancer Cells. *Nanoscale* **2014**, *6*, 11841-11855.

216 Goel, M.; Narasimha, K.; **Jayakannan, M.** Helical Self-assemblies of Segmented Poly(phenylenevinylene)s and their Hierarchical Donor-Acceptor Complexes. *Macromolecules* **2014**, *47*, 2592-2603.

217 Balamurugan, A.; Vikash Kumar; **Jayakannan, M.** Carboxylic Distilbene Fluorescent Polymer Chemosensor for Temperature, Metal-ion and Biomolecule. *Chem. Commun*. **2014,** *50*, 842-845.

218 Smita, K.; **Jayakannan, M.** Thermo-responsive and Shape Transformable Amphiphilic Scaffolds for Loading and Delivering Anticancer Drugs. *J. Mater. Chem. B*. **2014**, *2*, 4142-4152.

219 Surnar B.; Pramod, P. S.; **Jayakannan, M.** Biodegradable Block Copolymer Scaffolds for Loading and Delivering Cisplatin Anticancer Drug. *Z. Anorg. Allg. Chem., ZAAC)* (*Dedicated issue to Prof. CNR Rao's 80th Birthday*) **2014**, *640* (6), 1119-1126.

220 Thadke, S. A.; **Hotha, S.** Efficient Synthesis of Oligosaccharyl 1,2-*O*-orthoesters from *n*-pentenyl Glycosides and Application to the Pentaarabinofuranoside of the Mycobacterial Cell Surface. *Org. Biomol. Chem.* **2014**, 10.1039/C4OB01395F

221 Thadke, S. A.; Mishra, B.; **Hotha, S.** Gold(III)-Catalyzed Glycosidations for 1,2-trans and 1,2-cis Furanosides. *J. Org. Chem.* **2014**, *79*, 7358-7371.

222 Islam, M.; Tirukoti, N. D.; Nandi, S.; **Hotha, S.** Hypervalent Iodine Mediated Synthesis of *C-2 Deoxy* Glycosides and Amino Acid Glycoconjugates. *J. Org. Chem.* **2014,** *79*, 4470-4476.

223 Shaikh, A. Y.; Das, S.; Pati, D.; Dhaware, V.; Gupta, S. S.; **Hotha, S.** Cationic Charged Helical Glycopolypeptide Using Ring Opening Polymerization of 6-Deoxy-6-azido-glyco-N-carboxyanhydride. *Biomacromol.* **2014**, *15*, 3679-3686.

224 Sultane, P. R.; Mete, T. B.; **Bhat, R. G.** Chemoselective *N*-deacetylation Under Mild Conditions. *Org. Biomol. Chem*. **2014**, *12*, 261-264.

225 Ganesh Kumar, M.; Thombare, V. J.; Bhaisare, R. D.; Adak. A.; **Gopi. H. N.** Synthesis of Tetrasubstituted Symmetrical Pyrazines from β-keto γ-amino Esters: A Mild Strategy for Self-dimerization of Peptides. *Eur. J. Org. Chem.* **2014** (*accepted*).

226 Jadhav, S. V.; Misra, R.; **Gopi, H. N.** Foldamers to Nanotubes: Influence of Amino acid Side-chains in the Hierarchical Assembly of α, γ^4-Hybrid Peptide Helices *Chem. Eur.- J.* **2014** (*Accepted as Very Important Paper*) DOI: 10.1002/chem.201404961

227 Mali, S.M.; Ganesh Kumar, M.; Katariya, M. M.; **Gopi, H. N.** HBTU Mediated 1-hydroxy-benzotriazole (HOBt) Conjugate Addition: Synthesis and Stereochemical Analysis of β-benzotriazole *N*-oxide Substituted γ-amino acids and Hybrid Peptides. *Org. Biomol. Chem.* **2014**, 12, 8462.

228 Mali, S. M.; **Gopi. H. N.** Thioacetic acid/NaSH-mediated Synthesis of *N*-protected Amino Thioacids and Their Utility in Peptide Synthesis. *J. Org. Chem*. **2014,** *79,* 2377.

229 Bandyopadhyay, A.; **Malik, A.**; Kumar, M. G.; **Gopi, H. N.** Exploring β-Hydroxy γ-Amino Acids (Statines) in the Design of Hybrid Peptide Foldamers. *Org. Lett*. **2014**, *16*, 294.

230 Sabale, P. M.; George, J. T.; **Srivatsan, S. G.** Base-modified PNA-graphene Oxide Platform as a turn-On Fluorescence Sensor for the Detection of Human Telomeric Repeats. *Nanoscale* **2014**, *6*, 10460-10469.

231 Tanpure, A. A.; **Srivatsan, S. G.** Synthesis, Photophysical Properties and Incorporation of a Highly Emissive and Environment-sensitive Uridine Analogue Based on the Lucifer Chromophore. *ChemBioChem* **2014**, *15*, 1309-1316.

232 Sankar, R. K; Kumbhare, R. S.; Dharmaraja, A. T.; **Chakrapani, H.** A Phenacrylate Scaffold for Tunable Thiol Activation and Release *Chem. Commun.* **2014**, DOI: 10.1039/C4CC07343F

233 Sharma, K.; **Chakrapani, H.** Site-Directed Delivery of Nitric oxide to Cancers *Nitric Oxide Biol. Chem.* **2014**, DOI: 10.016/j.niox.2014.07.005.

234 Dharmaraja, A. T.; Jain, C.; **Chakrapani, H.** Substituent Effects on Reactive Oxygen Species (ROS) Generation by Hydroquinones. *J. Org. Chem.* **2014**, *79*, 9413-9417.

235 Malwal, S. R.; Labade, A.; Andhalkar, A.; Sengupta, K.; **Chakrapani, H.** A Highly Selective Sulfinate Ester Probe for Thiol Bioimaging. *Chem. Commun.* **2014**, *50*, 11533-11535.

236 Khodade, V. S.; Sharath Chandra, M.; Banerjee, A.; Lahiri, S.; Pulipeta, M.; Rangarajan, R.; **Chakrapani, H.** Bioreductively Activated Reactive Oxygen Species (ROS) Generators as MRSA Inhibitors. *ACS Med. Chem. Lett.* **2014**, 5, 777-781.

237 Dharamaraja, A. T; Ravikumar, G.; **Chakrapani, H.** Arylboronate Ester Based Diazeniumdiolates (BORO/NO), a Class of Hydrogen Peroxide Inducible Nitric Oxide (NO) Donors. *Org. Lett.* **2014**, *16*, 2610-2613.

238 Dharamaraja, A. T; **Chakrapani, H.** A Small Molecule for Controlled Generation of Reactive Oxygen Species (ROS). *Org. Lett.* **2014**, *16*, 398-401.

239 Kand, D.; Mandal, P. S.; Saha, T.; **Talukdar, P.** Structural Imposition on off-on Response of Naphthalimide Based Probes for Selective Thiophenol Sensing. *RSC Adv.* **2014**, DOI: 10.1039/C4RA09042J.

240 Deshmukh, S. C.; **Talukdar, P.** Stereoselective Synthesis of (2S,3R)-α-hydroxy-β-amino acids (AHBAs): Valinoctin A, *(2S,3R)*-3-amino-2-hydroxydecanoic Acid and a Fluorescent-labeled (2S,3R)-AHBA. *J. Org. Chem.* **2014, DOI:** 10.1021/jo501751u.

241 Saha, T.; Dasari, S.; Tewari, D.; Prathap, A.; Sureshan, K. M.; Bera, A. K.; **Mukherjee, A.; Talukdar, P.** Hopping-mediated Anion Transport Through a Mannitol-Based Rosette Ion Channel. *J. Am. Chem. Soc.* **2014,** *136*, 14128-14135.

242 Roy, A.; Kand, D.; Saha, T.; **Talukdar, P.** Pink Fluorescence Emitting Fluoride Ion Sensor: Investigation of the Cascade Sensing Mechanism and Bioimaging Applications. *RSC Adv.* **2014,** *4*, 33890-33896.

243 Saha, T.; Roy, A.; Gening, M. L.; Titov, D. V.; Gerbst, A. G.; Tsvetkov, Y. E.; Nifantiev, N. E.;

Talukdar, P. Cyclo-oligo-(1 → 6)-β-D-glucosamine Based Artificial Channels for Tunable Transmembrane Ion Transport. *Chem. Commun.* **2014,** *50*, 5514-5516.

244 Roy, A.; Kand, D.; Saha, T.; **Talukdar, P. A** Cascade Reaction Based Fluorescent Probe for Rapid and Selective Fluoride Ion Detection. *Chem. Commun.* **2014,** *50*, 5510-5513.

245 Kand, D.; Saha, T.; **Talukdar, P.** Off-on Type Fluorescent NBD-probe for Selective Sensing of Cysteine and Homocysteine Over Glutathione Sensor. *Actuat. B-Chem.* **2014,** *196*, 440-449.

246 Kand, D.; Mandal, P. S.; Datar, A.; **Talukdar, P.** Iminocoumarin Based Fluorophores: Indispensable Scaffolds for Rapid, Selective and Sensitive Detection of Thiophenol. *Dyes Pigments* **2014,** *106*, 25-31.

247 Roy, A.; Datar, A.; Kand, D.; Saha, T.; **Talukdar, P.** A Fluorescent off-on NBD-probe for F-sensing: Theoretical Validation and Experimental Studies. *Org. Biomol. Chem.* **2014,** *12*, 2143-2149.

248 Chauhan, D. P.; Saha, T.; Lahiri, M.; **Talukdar, P.** BODIPY Based 'click on' Fluorogenic Dyes: Application in Live Cell Imaging. *Tetrahedron Lett.* **2014,** *55*, 244-247.

249 Chauhan, D. P.; Varma, S. J.; Vijeta, A.; Banerjee, P.; **Talukdar, P.** A 1,3-Amino group Migration Route to form Acrylamidines. *Chem. Commun.* **2014,** *50*, 323-325.

250 Khan, S.; Adak, A.; Murthy, R. V.; **Kikkeri, R.** Recent Advances in the Metallo-Glycodendrimers and its Potential Applications. *Inorg. Chem. Acta*. **2014**, 406, 26-33.

251 Chaudhary, P. M.; Murthy, R. V.; **Kikkeri, R.** Advances and Prospects of Sugar Capped Quantum Dots. *J. Mat. NanoSci*. **2014**, 1, 7-11.

252 Ravikiran C.G.; **Jeganmohan, M.** Ruthenium Catalyzed Ortho-arylation of Acetanilides with Aromatic Boronic Acids: An Easy Route to Prepare Phenanthridines and Carbazoles. *Chem. Commun.* **2014,** *50*, 2442.

253 Manikandan R.; **Jeganmohan, M.** Ruthenium Catalyzed Dimerization of Propiolates: A Simple Route to α-Pyrones. *Org. Lett.* **2014,** *16*, 652.

254 Manikandan R.; **Jeganmohan, M.** Ruthenium-Catalyzed Hydroarylation of Anilides with Alkynes: An Efficient Route to *Ortho*-Alkenylated Anilines. *Org. Lett.* **2014,** *16*, 912.

255 Kishor P.; **Jeganmohan, M.** *ortho*-Benzoxylation of N-Alkyl Benzamides with Aromatic Acids Catalyzed by Ruthenium(II) Complex. *Chem. Eur. J.* **2014,** *20*, 4092.

256 More N. Y; **Jeganmohan, M.** Aerobic Dehydrogenative α-Diarylation of Benzyl Ketones with Aromatics through Carbon-Carbon Bond Cleavage. *Org. Lett.* **2014,** *16*, 804.

257 Manikandan R.; **Jeganmohan, M.** Ruthenium-Catalyzed Cyclization of Anilides with Substituted Propiolates or Acrylates: An Efficient Route to 2-Quinolinones. *Org. Lett.* **2014,** *16*, 3568.

258 Pimparkar S.; **Jeganmohan, M.** Palladium-catalyzed cyclization of benzamides with Arynes: Application to the Synthesis of Phenaglydon and *N*-Methylcrinasiadine. *Chem. Commun.* **2014,** *50*, 12116.

259 Reddy, M. C.; **Jeganmohan, M.** Ruthenium-catalyzed Cyclization of Aromatic Nitriles with Alkenes: Stereoselective Synthesis of (Z)-3-methyleneisoindolin-1-ones. *Org. Lett.* **2014,** *16*, 4866.

260 Kishor P.; **Jeganmohan, M.** Ruthenium-catalyzed Highly Regio- and Stereoselective Hydroarylation of Aromatic Sulfoxide with Alkynes via C-H bond Activation. *Chem. Commun.* **2014,** *50*, 14573 (Highlited in *Synfacts* **2014,** 10, 1172).

261 More, N. Y.; **Jeganmohan, M.** A Regioselective Synthesis of Benzopinacolones via Aerobic Dehydrogenative α-Arylation at Tertiary sp^3 C-H Bond of 1, 1-Diphenylketones with Aromatics and Heteroaromatics. *Chem. Eur. J.* **2014,** *(in press).*

262 Pimparkar S.; Kishor P.; **Jeganmohan, M.** Ruthenium(II)-Catalyzed *ortho* C-O Bond formation of Substituted Aromatics with Oxygen Nucleophiles through C-H Bond Activation (invited review). *Proc Indian Natn Sci Acad.* **2014,** *(in press).*

263 Palvai, S.; Nagraj, J.; Mapara, N.; Chowdhury, R.; **Basu, S.** Dual Drug Loaded Vitamin D3 Nanoparticle to Target Drug Resistance in Cancer. *RSC Adv.* **2014**, DOI: 10.1039/C4RA06475E.

264 **Kalia, J.**; Milescu, M.; Salvatierra, J.; Wagner, J.; Klint, J. K.; King, G. F.; Olivera, B. M.; Bosmans, F. From Foe to Friend: Using Animal Toxins to Investigate Ion Channel function. *J. Mol. Biol*. **2014**, doi: 10.1016/j.jmb.2014.07.027.

265 Gilchrist, J., Dutton, S., Diaz-Bustamante, M., McPherson, A., Olivares, N., **Kalia J.**, Escayg, A., and Bosmans, F. Nav1.1 Modulation by a Novel Triazole Compound Attenuates Epileptic Seizures in Rodents. *ACS Chem. Biol*. **2014**, *9*, 1204-1212.

266 Gopalakrishna, T. Y.; Reddy J. S.; **Anand V. G.** An Amphoteric Switch to Aromatic and Antiaromatic States of a Neutral Air-Stable 25πRadical. *Angew. Chem. Int. Ed*. **2014**, *53*, 10984.

267 Gopalakrishna T. Y.; **Anand V. G.** Reversible Redox Reaction between Antiaromatic and Aromatic States of 32π-Expanded Isophlorins. *Angew. Chem. Int. Ed*. **2014**, *53*, 6678.

268 Nagarkar, S. S.;Saha, T.;Desai, A. V.; **Talukdar, P.; Ghosh. S. K.** Metal-Organic Framework Based Highly Selective Fluorescence *Turn-on* Probe for Hydrogen Sulphide *Sci. Rep. 2014,* (Just accepted).

269 Joarder, B.; Desai, A. V.; Samanta, P.; Mukherjee, S.; **Ghosh, S. K.** Selective and Sensitive Aqueous Phase Detection of TNP (2,4,6- trinitro phenol) by an Amine Functionalized Metal-Organic Framework *Chem. Eur. J. 2014, (Just accepted).*

270 Joarder, B.; Mukherjee, S.; Chaudhari, A. K.; Desai, A. V.; Manna, B.; Ghosh, S. K. Guest-Responsive Function of a Dynamic Metal-Organic Framework with π-Lewis Acidic Pore Surface *Chem. Eur. J. 2014, 20, 15303-15308. (Just accepted).*

271 Mukherjee, S.; Joarder, B.; Manna, B.; Desai, A. V.; Chaudhari, A. K.; **Ghosh, S. K.** Framework-Flexibility Driven Selective Sorption of *p*-Xylene over Other Isomers by a Dynamic Metal-Organic Framework *Sci. Rep.* **2014**. DOI:10.1038/srep05761

272 Manna, B.; Joarder, B.; Desai, A. V.; Karmakar, A.; **Ghosh, S. K.** Anion-Responsive Tunable Bulk Phase Homochirality and Luminescence of a Cationic Framework. *Chem. Eur. J.* **2014**, *20*, 12399–12404.

273 Joarder, B.; Mukherjee, S.; Xue, S.; Tang, J.; **Ghosh S. K.** Structures and Magnetic Properties of Two Analogous Dy_6 Wheels with Electron-Donation and -Withdrawal Effects. *Inorg. Chem.* **2014**, *53*, 7554–7560.

274 S. S.; Desai, A. V.; **Ghosh, S. K.** Fluorescent Metal-Organic Framework for Highly Selective Detection of Nitro Explosive in Aqueous Phase Nagarkar. *Chem. Commun.* **2014**, *50*, 8915-8918.

275 Nagarkar, S. S.; Desai, A. V.; **Ghosh, S. K.** Stimulus-Responsive Metal-Organic Frameworks. *Chem. Asian J.* **2014**, *9*, 2358–2376.

276 Nagarkar, S. S.; Unni, S. M.; Sharma, A.; Kurungot, S.; **Ghosh, S. K.** Two-in-one: Inherent Anhydrous and Water-assisted High Proton Conduction in a 3D Metal-Organic Framework. *Angew. Chem. Int. Ed.* **2014**, *53*, 2638-2642.

277 Chaudhari, A. K.; Sharma, A.; Mukherjee, S.; Joarder, B.; **Ghosh, S. K.** Capsule Voided Nanospace Confinement in a π-Stacked Supramolecular Organic Solid. *CrystEngComm* **2014**, *16*, 4691-4695. (Invited Article)

278 Manna, B.; Singh, S.; **Ghosh, S. K.** Guest Driven Structural Transformation Studies of a Luminescent Metal-Organic Framework. *J.Chem. Sci.* **2014**, *126*, 1417-1422. (Just accepted). (Invited Article)

279 Mukherjee, S.; Joarder, B.; Xue, S.; Tang, J.; **Ghosh, S. K.** Slow Magnetic Relaxation in an Asymmetrically Coupled Heptanuclear Dysprosium(III)-Nickel(II) Architecture. *Proc. Natl. Acad. Sci., India, Sect. A Phys. Sci.* **2014**, *84*, 151-156.

280 Nagarkar, S. S.; **Ghosh, S. K.** Reversible Structural Transformations in a Co(II) Based 2D Dynamic Metal-Organic Framework Showing Selective Solvent Uptake *J. Chem. Sci.* **2014**, (Just accepted). (Invited Article)

281 Agarwal, R. A.; Mukherjee, S.; Sañudo, E. C.; **Ghosh, S. K.;** Bharadwaj P. K. Gas Adsorption, Magnetism, and Single-Crystal to Single-Crystal Transformation Studies of a Three-Dimensional Mn(II) Porous Coordination Polymer. *Cryst. Growth Des*. **2014**, 5585-5592.

282 Mukherjee, S.; **Ghosh, S. K.** Recent Progress in the Realm of Homonuclear Ln_6 Single Molecule Magnets: Structural Overview and Synthetic Approaches. Proceedings of the Indian National Science Academy, 2014, (Just accepted). (Invited Article)

283 Manna, B.; Singh, S.; Karmakar, A.; Desai, A. V.; **Ghosh, S. K.** Selective Anion Exchange and Tunable Luminescent Behaviors of MOF based Supramolecular Isomers. *Inorg. Chem.* **2014**, (Just accepted).

284 Srivastava, A. K.; Praveen Kumar, B.; Mahawar, I. K.; Divya, P.; Shalini, S.; **Boomishankar, R.** Anion Driven $[Cu^{II}L_2]_n$ Frameworks: Crystal Structures, Guest-Encapsulation, Dielectric, and Possible Ferroelectric Properties. *Chem. Mater.* **2014**, *26*, 3811-3817.

285 Yadav, A.; Srivastava, A. K.; Balamurugan, A.; **Boomishankar, R.** A Cationic Copper(I) Iodide Cluster MOF Exhibiting Unusual Ligand Assisted Thermochromism. *Dalton Trans.* **2014**, 43, 8166-8169.

286 Gupta, A. K.; Srivastava, A. K.; Mahawar, I. K.; **Boomishankar, R.** Discrete and Polymeric Cu(II) Complexes Derived from in Situ Generated Pyridyl-Functionalized Bis(amido)phosphate Ligands, $[PO_2(NHPy)_2]^-$. *Cryst. Growth Des.* **2014**, *14*, 1701-1709 *(appeared as spotlight article).*

287 Gupta, A. K.; Yadav A.; **Boomi Shankar,** R. Discrete and Polymeric Coordination Assemblies Derived from 3-Pyridyl Attached Flexible Phosphoric Triamide Ligand and Copper Salts. *Proc. Nat. Acad. Sci., India Sec. A: Phy. Sci.* **2014**, *84*, 205-212 (invited for a special issue celebrating the international year of crystallography).

288 Gupta, A. K.; Srivastava, A. K.; **Boomishankar, R.** A Tetrakis(amido)phosphonium Cation Containing 2-pyridyl (^{2}Py) Substituents, $[P(NH^2Py)_4]^+$, and its Reactivity Studies with Ag(I) salts. *J. Chem. Sci.* **2014**, 0000 (special issue of MTIC-XV conference).

289 Chaturvedi, S.; Sarkar, I.; Shirolkar, M. M.; Jeng, U.-S.; Yeh, Y. Q.; Rajendra, R.; **Ballav, N.;** Kulkarni, S. Probing Bismuth Ferrite Nanoparticles by Hard X-Ray Photoemission: Anomalous Occurrence of Metallic Bismuth. *Applied Physics Letters* **2014**, *105*, 102910.

290 Dhara, B.; Patra, P. P.; Jha, P. K.; Jadhav, S. V.; Pavan Kumar, G.; **Ballav, N.** Redox-Induced Photoluminescence of Metal–Organic Coordination Polymer Gel. *The Journal of Physical Chemistry C* **2014**, *118*, 19287-19293.

291 Chaturvedi, S.; Shirolkar, M. M.; Rajendra, R.; Singh, S.; **Ballav, N.;** Kulkarni, S. Coercivity and Exchange Bias of Bismuth Ferrite Nanoparticles Isolated by Polymer Coating. *Journal of Applied Physics* **2014**, *115*, 123906.

292 Jha, P. K.; Dhara, B.; **Ballav, N.** Nanofibers to Nanocuboids of Polyaniline by Lead Nitrate: Hierarchical Self-Assembly with Lead Ions. *RSC Advances* **2014**, *4*, 9851-9855.

293 Koninti, R. K.; Sengupta, A.; Gavvala, K.; **Ballav, N.; Hazra, P.** Loading of an Anti-Cancer Drug onto Graphene Oxide and Subsequent Release to DNA/RNA: A Direct Optical Detection. *Nanoscale* **2014**, *6*, 2937-2944.

294 Koninti, R. K.; Sengupta, A.; Gavvala, K.; **Ballav, N.; Hazra, P.** An Anticancer Drug to Probe Non-Specific Protein–DNA Interactions. *Physical Chemistry Chemical Physics* **2014**, *16*, 3914-3917.

295 Shyamapada, N.; **Vaidhyanathan, R. J.** Tuning porosity via control of interpenetration in a zinc isonicotinate metal organic framework *Chem. Sci*. **2014**, DOI:10.1007/s12039-014-0680-2

296 **Verma, S.;** Kumar, A.; Pravarthana, D.; Deshpande, A.; Ogale, S. B.; Yusuf, S. M. Off-Stoichiometric Nickel Cobaltite Nanoparticles: Thermal Stability, Magnetization, and Neutron Diffraction Studies. *J. Phys. Chem. C* **2014,** *118*, 16246-16254.

297 Gogia, S.; **Puranik, M.** Solution Structures of Purine Base Analogues 6-chloroguanine, 8-azaguanine and Allopurinol. *J. Biomol. Struc. Dyn*. **2014**, 32, 27-35.

298 Milan-Garces, E. A.; Mondal, S; Udgaonkar, J. B.; **Puranik, M.** Intricate Packing in the Hydrophobic Core of Barstar through a CH-pi Interaction. *J. Raman Spectrosc.* **2014**, DOI 10.1002/jrs.4558.

299 Ramachandran, G.; Erix A. Milan-Garces, E. A.; Udgaonkar, J. B.; **Puranik, M.** Resonance Raman Spectroscopic Characterization of the Kinetics of Tau Fibril Formation. *Biochem*. **2014**, DOI: 10.1021/bi500528x.

300 Kumar, S.; Singh, S. K.; Calabrese, C.; Maris, A.; Melandri, S.; **Das, A.** Structure of Saligenin: Microwave, UV and IR Spectroscopy Studies in a Supersonic Jet Combined with Quantum Chemistry Calculations. *Phys. Chem. Chem. Phys.* **2014,** *16*, 17163-17171.

301 Hill, J. G.; **Das, A.** Interaction in the Indole...Imidazole Heterodimer: Structure, Franck-Condon Analysis and Energy Decomposition. *Phys. Chem. Chem. Phys.* **2014,** *16*, 11754-11762.

302 Singh, S. K.; Kumar, S.; **Das, A.** Competition between $n \rightarrow \pi^*$ and Conventional Hydrogen Bonding (N-H...N) Interactions: An Ab Initio study of the Complexes of 7-Azaindole and Fluorosubstituted Pyridines. *Phys. Chem. Chem. Phys.* **2014,** *16*, 8819-8827.

303 Kumar,V.; Sengupta, A.; Gavvala, K.; Koninti, R. K.; **Hazra, P.** Spectroscopic and Thermodynamic Insights into the Interaction Between Proflavine and Human Telomeric G-Quadruplex DNA. *J. Phys. Chem. B* **2014**, *118*, 11090–11099.

304 Sengupta, A.; Gavvala, K.; Koninti, R. K.; **Hazra, P.** Role of Mg^{+2} Ions in Flavin Recognition by RNA Aptamer. *J. Photochemistry and Photobiology B: Biology* **2014**, *140*, 240-248.

305 Koninti, R. K.; Gavvala, K.; Sengupta, A.; **Hazra, P.** Excited State Proton Transfer Dynamics of Topotecan Inside Bio-mimicking Nano-Cavity. *J. Phys. Chem. B* **2014**, ASAP, DOI: 10.1021/jp5066902.

306 Saha, T.; Sengupta, A.; **Hazra, P.**; Talaukdar, P. *In vitro* Sensing of Cu^{+} through a Green Fluorescence Rise of Pyranine. *Photochem. Photobiol. Sci.* **2014**, **13**, 1427-1433.

307 Gavvala, K.; Koninti, R. K.; Sengupta, A.; **Hazra, P.** Excited State Proton Transfer Dynamics of an Eminent Anticancer Drug, Ellipticine, in Octyl Glucoside Micelle. *Phys. Chem. Chem. Phys.* **2014**, *16*, 14953-14960.

308 Sengupta, A.; Singh, R. K.; Gavvala, K.; Koninti, R. K.; **Mukherjee, A.; Hazra, P.** Urea Induced Unfolding Dynamics of Flavin Adenine Dinucleotide (FAD): Spectroscopic And Molecular Dynamics Simulation Studies from Femto-second to Nano-Second Regime. *J. Phys. Chem. B* 2014, *118*, 1881-1890.

309 Gavvala, K.; Koninti, R. K.; Sengupta, A.; **Hazra, P.** Cucurbit [7] Uril Assisted Ultraviolet to Visible Fluorescence Switch of a Heart Medicine. *Phys. Chem. Chem. Phys.* 2014, *16*, 2823-2826.

310 Koninti, R. K.; Sengupta, A.; Gavvala, K.; Ballav, N.; **Hazra, P.** Loading of an Anti-Cancer Drug onto Graphene Oxide and Subsequent Release to DNA/RNA: A Direct Optical Detection. *Nanoscale* **2014**, *6*, 2937-2944.

311 Sengupta, A.; Gavvala, K.; Koninti, R. K.; Ballav, N.; **Hazra, P.** An Anticancer Drug to Probe Non-specific Protein-DNA Interactions. *Phys. Chem. Chem. Phys.* 2014, *16*, 3914-3917.

312 Gavvala, K.; Sengupta, A.; Koninti, R. K.; **Hazra, P.** Femtosecond to Nanosecond Dynamics of 2, 2-Bipyridine-3,3-diol Inside the Nano-Cavities of Molecular Containers. *Phys. Chem. Chem. Phys.* 2014, *16*, 933-939.

313 Joshi, H.; Sengupta, A.; Gavvala, K.; **Hazra, P.** Unraveling the Mode of Binding of the Anticancer Drug Topotecan with ds-DNA. *RSC Advances* **2014**, *4*, 1015-1024.

314 **Nag, A.**; Zhang, H.; Janke, E.; Talapin, D. V. Inorganic Surface Ligands for Colloidal Nanomaterials. *Z. Phys. Chem.* **2014** (accepted)

315 Tandon, B.; Shanker, G. S.; **Nag, A.** Multifunctional Sn- and Fe-Codoped In2O3 Colloidal Nanocrystals: Plasmonics and Magnetism. *J. Phys. Chem. Lett.* **2014**, *5*, 2306 – 2311.

316 **Nag, A.**; Kundu, J.; Hazarika, A. Seeded-Growth, Nanocrystal-Fusion, Ion-Exchange and Inorganic-Ligand Mediated Formation of Semiconductor Based Colloidal Heterostructured Nanocrystals. *CrystEngComm* **2014**, *16*, 9391-9407

317 Swarnkar, A.; Shanker, G. S.; **Nag, A.** Organic-Free Colloidal Semiconductor Nanocrystals as Luminescent Sensors for Metal Ions and Nitroaromatic Explosives. *Chem Commun* **2014**, *50*, 4743-4746.

318 Kadlag, K. P.; Patil, P.; Rao, M. J.; Datta, S.; **Nag, A.** Luminescence and Solar Cell from Ligand-Free Colloidal $AgInS_2$ Nanocrystals. *CrystEngComm* **2014**, 16, 3605-3612.

319 Rao, M. J.; Shibata, T.; Chattopadhyay, S.; **Nag, A.** Origin of Photoluminescence and XAFS Study of $(ZnS)_{1-x}(AgInS_2)_x$ Nanocrystals. *J. Phys. Chem. Lett.* **2014**, *5*, 167-173.

320 **Chugh, J.** Determining Transient Nucleic Acid Structures by NMR. *Chemical Biology of Nucleic Acids: RNA Technologies*. (Ed) Erdmann V. A.; Markiewicz W. T.; Barciszewski. *J. Springer* **2014**, 181-198 (Book Chapter)

321 Sunda A. P.; Dhavale V. M.; Sreekumar K.; **Venkatnathan A.** Structure and Dynamics of Benzyl-NX_3 (X = Me, Et) Trifluoromethanesulfonate Ionic Liquids. *J. Phys. Chem. B* **2014**, *118*, 1831-1838.

322 More M.; Sunda A. P.; **Venkatnathan A.** Polymer Chain Length, Phosphoric Acid Doping and Temperature Dependence on Structure and Dynamics of ABPBI [poly(2,5-benzimidazole)] Polymer Electrolyte Membrane. *RSC Advances* **2014**, *4*, 19746-19755.

323 Ramya K. R.; Kumar R.; **Venkatnathan A.** Energy and Spectral Characteristics of Hydrogen Occupied Pure and Tetrahydrofuran Doped Water Cages. *Comp. Theo. Chem.* **2014**, *1039*, 28-32.

324 Ramya K. R.; Kumar P.; Kumar A.; **Venkatnathan A.** Interplay of Phase Separation, Tail Aggregation, and Micelle Formation in the Nanostructured Organization of Hydrated Imidazolium Ionic Liquid. *J. Phys. Chem. B* **2014**, *118*, 8839-8847.

325 Sasikala, W. D.; **Mukherjee, A.** Single Water Entropy: Hydrophobic Crossover and Application to Drug Binding. *J. Phys. Chem. B* **2014**, *118* (36), 10553-10564.

326 Varghese, A.;**Ghosh, P.;** Datta, S. Cadmium Vacancy Minority Defects as Luminescence Centers in Size and Strain Dependent Photoluminescence Shifts in CdS Nanotubes. *J. Phys. Chem. C* **2014**, *118*, 21604 - 21613.

327 Joshi, S.; Shukla A.; Katiyar H.; **Hazra A.** Mahesh T. S. Estimating Franck-Condon Factors Using an NMR Quantum Processor. *Phys. Rev. A* **2014,** *90*, 022303.

328 **Chaudhury S.** Poisson Indicator and Fano Factor for Probing Dynamic Disorder in Single Molecule Enzyme Inhibition Kinetics. *J. Phys. Chem. B* **2014**, 118, 10405–1041.

External Research Grants

Sr. No.	Name of the Project	Project Leader	Sanctioning Authority	Period (From - to)	Sanctioned amount (Rs. in lakhs) ₹
1	Material for Optoelectronics: Design, synthesis and of hybrid conjugated molecules with luminescent properties	Dr. V.G. Anand	DST	24-01-2006 to 31-09-2009	3.00
2	Development of electricity conducting polyanilinc nanomaterial	Dr. M. Jayakannan	DST	31-03-2008 to 30-03-2011	44.38
3	Modeling and simulation of polymer electrolyte membranes and molecular transport in fuel cells	Dr. Arun Venkatnathan	DST - SERB	12-03-2010 to 11-03-2013	26.37
4	Photoinduced electron transfer rate (between flavins and aromatic aminoacids) in nanocavity of proteins versus bulk waters	Dr. Partha Hazra	DST - SERB	23-03-2010 to 22-03-2013	16.44
5	Functionalized ribonucleoside analogues: Synthesis, site-specific enzymatic incorpora -tion and applications	Dr. Seerghazhi G. Srivatsan	DST - SERB	26-03-2010 to 25-03-2013	35.46
6	Development of green chemical melt transuretane reaction for polyurethanes	Dr. M. Jayakannan	DST - SERB	20-04-2010 to 19-04-2013	36.19
7	Investigation of gamma and hybrid gamma helical peptides as HIV-I fusuin inhibitors	Dr. Hosahudya Gopi	DST - SERB	20-04-2010 to 19-04-2013	33.90
8	Organic sources of gasesous entities with physiological relevance	Dr. Harinath Chakrapani	DST - SERB	07-03-2011 to 06-03-2014	26.00

Sr. No.	Name of the Project	Project Leader	Sanctioning Authority	Period (From - to)	Sanctioned amount (Rs. in lakhs) ₹
9	Design and synthesis of functional framework materials based on P-N and P-O building blocks	Dr. R. Boomishankar	DST - SERB	31-12-2008 to 30-12-2011	19.68
10	Carbohydrate capped nanoparticles as tumor specific drug delivery systems	Dr. Raghavendra Kikkeri	DST and Max Planck Gesellschaft (DST-MPG)	01-04-2011 to 01-04-2014	37.27
11	Development and functional studies of homochiral inorganic - organic hybrid materials	Dr. Sujit K. Ghosh	DAE	16-08-2011 to 15-08-2014	16.44
12	Chiral lanthanide carbohydrate clusters for studying carbohydrate - protein interactions	Dr. Raghavendra Kikkeri	DAE	16-08-2011 to 15-08-2014	16.16
13	Total synthesis of natural benzo(c) phenanthridine alkaloids by metal-catalyzed cyclization or C-H bond activation reaction as a key step	Dr. Masilamani Jeganmohan	DAE	16-08-2011 to 15-08-2014	16.99
14	Directed assembly of poly-nuclear Ru (II) complexes on carbon nanostructures : A prospective organic photovoltaic cells	Dr. Raghavendra Kikkeri	DST - SERB	27-09-2011 to 26-09-2013	19.44
15	Study of transmembrane ion channel activity of cyclo-(1-6) -B-D-glucosamine derivatives and evaluation of their antibacterial potential	Dr. Pinaki Talukdar	DST - SERB	29-09-2011 to 28-09-2013	13.92
16	New insight of flavin-aptamer recognition process with the help of biophysical studies	Dr. Partha Hazra	CSIR	01-01-2012 to 31-12-2014	6.70
17	Conformation of microhydrated peptides: Laser-desorption jet-cooled studies	Dr. Aloke Das	DST - SERB	01-03-2012 to 28-02-2015	39.60

Sr. No.	Name of the Project	Project Leader	Sanctioning Authority	Period (From - to)	Sanctioned amount (Rs. in lakhs) ₹
18	Two-dimensional metal - organic coordination networks	Dr. Nirmalya Ballav	DAE	05-03-2012 to 04-03-2015	17.00
19	Application of the chemistry lab skills teaching resources to the Indian education system	Dr. Harinath Chakrapani	BC	01-01-2012 to 31-12-2012	3.10
20	Collaboration in medical chemistry between IISER Pune and Keele University, UK under UKIERI Programme	Prof. K.N. Ganesh	British Council Division	01-04-2012 to 31-03-2013	8.15
21	Palladium catalyzed chelation assisted C-H bond functionalization of aromatics, alkenes and alkanes	Dr. M. Jeganmohan	DST - SERB	03-07-2012 to 02-07-2015	45.99
22	Functional studies of novel inorganic-organic hybrid frameworks with guest accessible sites	Dr. Sujit Kumar Ghosh	DST - SERB	05-07-2012 to 04-07-2015	24.76
23	Development and application of theoretical methods for mechanistic understanding of ultrafast photoinduced molecular processes	Dr. Anirban Hazra	DST - SERB	03-08-2012 to 02-08-2015	23.90
24	Enovex Technology Ltd	Dr. R. Vaidhyanathan	Enovex-IISER Pune Agreement	01-04-2012 to Open Ended	112.84
25	Redox-directed mycobacterial therapeutics	Dr. Harinath Chakrapani	DBT	28-09-2012 to 27-09-2015	56.70
26	Ramanujan Fellowship	Dr. Angshuman Nag	DST-SERB	29-10-2012 to 28-10-2017	73.00
27	Fluorescent nucleoside based amphiphiles: Synthesis, self assembly properties and applications	Dr. Seerghazhi G. Srivatsan	CSIR	01-11-2012 to 30-10-2015	12.00
28	FIST Program-2012 [48]	Prof. K.N. Ganesh	DST	07-01-2013 to 06-01-2018	500.00

Sr. No.	Name of the Project	Project Leader	Sanctioning Authority	Period (From - to)	Sanctioned amount (Rs. in lakhs) ₹
29	Dynamical effects in the mechanism of intercalation of anti-cancer drugs	Dr. Arnab Mukherjee	DST - SERB	13-06-2013 to 12-06-2016	54.75
30	Peripherally functionalized siloxane scaffolds for the assembly of multi-metallic cages, clusters and supramolecules	Dr. R. Boomishankar	DST - SERB	13-06-2013 to 12-06-2016	53.00
31	Design, synthesis and characterization of modified dipyrrins and its complexes	Dr. V.G. Anand	DST - SERB	17-6-2013 to 16-6-2016	50.00
32	Studies on non-covalent modulation of gating and selectivity of synthetic ion channels	Dr. Pinaki Talukdar	DST - SERB	1-7-2013 to 30-6-2016	52.00
33	Molecular modelling and simulation of nanostructure and dynamics of ionic liquid doped polymer electrolyte membrane fuel cells	Dr. Arun Venkatnathan	DST - SERB	05-09-2013 to 04-09-2016	55.00
34	Engineering novel supramolecular nanoplatform for paclitaxel delivery in cancer	Dr. Sudipta Basu	DST - SERB	06-09-2013 to 05-09-2016	24.48
35	Ligand-free colloidal all-inorganic semiconductor nanocrystals: Synthesis, photophysics and optoelectronic application	Dr. Angshuman Nag	DST - SERB	30-12-2013 to 29-12-2016	25.00
36	Glycochemical studies of mycobacterial arabinomycolate	Dr. Srinivas Hotha	IFCPAR	01.04.2014 to 31.3.2017	61.80
37	Synthesis of new fluorinated tumor-associated glycopeptide antigens and menningitis vaccine A analogues	Madhuri Vangala	DST - SERB	23-05-2014 to 22-05-2017	27.60
38	Development and functional studies of metal-organic polyhedras (MOPs)	Dr. Sujit Kumar Ghosh	INSA	13-05-2014 to 12-04-2017	5.00

Sr. No.	Name of the Project	Project Leader	Sanctioning Authority	Period (From - to)	Sanctioned amount (Rs. in lakhs) ₹
39	Design and development of amino acid based polymer scaffolds for drug delivery	Dr. M. Jayakannan	DST - SERB	04-08-2014 to 03-08-2017	102.00
40	CoE FAST	Prof. K.N. Ganesh	MHRD	01-10-2014 to 30-09-2019	400.00
41	Porphyrin, chlorin and isophlorin based near infrared dyes for high-efficiency dye-sensitized solar cells: an inspiration from nature (Indo-Singapore)	Dr. V.G. Anand	DST - SERB	30-08-2014 to 29-08-2017	43.67
42	Introduction of silylene in frustrated Lewis pair chemistry and their reactivity towards small molecules	Dr. Shabana Khan	DST - SERB	18-09-2014 to 17-09-2017	44.30
43	Ruthenium-catalysed meta selective C-H Bond functionalization of substituted aromatics	Dr. M. Jeganmohan	CSIR	01-10-2014 to 30-09-2014	9.00
44	Ruthenium catalyzed highly regio- and stereoselective oxidative coupling of Π-components: A versatile route to substitute alkenes, dienes and heterocycles	Dr. M. Jeganmohan	INSA	01-11-2014 to 31-10-2017	5.00
45	Design and synthesis of covalent and non-covalent composites from aromatic and antiaromatic macrocycles for molecular diode (Swarnajayanti Fellowship)	Dr. V.G. Anand	DST - SERB	03-11-2014 to 02-11-2019	195.21
	Total				**2493.2**

Conferences, Symposia and Events

Inter-IISER Chemistry Meet

December 22-23, 2008

IISER Pune organized a two-day meet with the main objective of bringing all faculty members in chemistry in all IISERs together to establish professional contacts, exchange their scientific ideas and to share their teaching experiences. The first Inter IISER Chemistry Meet started with Prof. C.N.R. Rao's plenary talk on "Novel Chemistry with Nanomaterials".

Visit of IISER delegation to University of Goettingen, Germany

December 9-12, 2010

A group of faculty from Chemistry group of IISER Pune, led by Dr. KN Ganesh, Director, visited University of Goettingen to participate in a 3-day seminar on Bioinspired Chemistry: from assembly to function. The German side consisting of eight faculty from the Institute of organic and biomolecular chemistry of Goettingen University was led by Prof U Diederschen, the Director of the host institute. The objective of the workshop was to understand each other's research interests and establish an international research and training group (IRTG) as envisaged by the Deutsche Forschung Gemeinschaft (DFG) in Bioorganic Chemistry. All aspects of bioorganic chemistry ranging from oligonucleotides, peptides /proteins etc. were discussed and many complementary areas could be identified for future collaboration.

Max Planck Partner Group in Glyconano-technology

November 14, 2011

The Max Planck Partner Group in Glyconano-technology has been sanctioned with Dr. Raghavendra Kikkeri as the head at the Indian side and Prof. Peter H. Seeberger as the Head at the German side. The partnership is aimed to further collaboration in carbohydrate research at IISER Pune and MPI of Colloids and Interfaces. The research in this project will focus on engineering of multifunctional

nanoparticles that will exploit biological processes to guide the carbohydrate mediated targeting, self assembly and remote actuation of nanoparticles to treat tumours in mouse models of cancer. The centre was formally inaugurated by Prof. P.H. Seeberger on 14 Nov 2011.

Mini-symposium on Chemical Biology

November 14, 2011

To coincide with the Inauguration of the MPI Partner Group in Glyco-nanotechnology, a one-day mini-symposium was organized on November 14, 2011. There were three sessions chaired by Prof. K.N. Ganesh, Prof. Ulf Diederichsen and Prof. Mike Blackburn. The speakers in this symposium were Prof. Peter H. Seeberger (Carbohydrate-based Nanotechnology), Sanjeev Galande (Chromatin organiser SATB1 as a molecular target for anticancer therapy), Dilip Dhavale (Fused, constrained and spiro iminosugars: Synthesis, glycosidase inhibitory and immunomodulatory activity study), Dipankar Chatterjee (Inhibitors of transcription and rescuing a drugged RNA polymerase), Raghavendra Kikkeri (Carbohydrate embedded Fe(III) complexes as biomimetic siderophores), Mike Blackburn (Recent advances in enzyme catalyzed phosphoryl transfer), Rajesh Gokhale (Systems-based analysis of chemical complexity and metabolic diversity), Harinath Chakrapani (Controlled generation of biologically reactive sulphur and oxygen species for therapeutic applications), Aurnab Ghose (Forming neuronal circuits: the role of extracellular matrix molecules), Souvik Maiti (Silencing of microRNAs with antagomirzymes and small molecules), Ulf Diederichsen (Building with peptide secondary structures), G.J. Sanjayan (From peptides to foldamers: Non-covalent interactions in structural design), H.N. Gopi (Design and conformational studies of functionalizable hybrid peptides), Saikrishnan Kayarat (Structural studies on motor-driven protein machines), S.G. Srivatsan (Synthesis, incorporation and applications of functionalized ribonucleoside analogues).

Mini Symposium on Materials

December 21, 2011

A one-day Mini Symposium on Novel Materials was held on December 21, 2011 and a dozen experts have presented their work related to the theme of the meeting. Prof. Ganesh, Director, IISER Pune welcomed the gathering and offered comments. The Inaugural lecture was given by Prof. P.V. Kamat, Radiation Laboratory, University of Notre Dame on "Nanostructure assemblies for solar energy conversion" followed by talks by speakers from IISER Thiruvananthapuram, NCL, Pune; BARC, Mumbai; and IISER Pune.

Mini-Symposium on Mass Spectrometry in Chemistry and Biology

March 12, 2012

The Mass Spectrometry Facility at the Institute was inaugurated on 12 March 2012 by Dr. Sourav Pal (Director, NCL). On this occasion a one-day mini-symposium on Mass Spectrometry in Chemistry and Biology was organized. The speakers in this symposium were:

Dr. Pradeep Thalappil - Advanced Mass Spectrometry to understand Nanomaterials

Dr. Aloke Das- Gas Phase Electronic and Vibrational Spectroscopy in a Jet-cooled Laser Desorption Time of Flight Mass Spectrometer

Dr. Ramakrishnan Nagaraj – Mass Spectrometry: Friend or Foe for Protein

Dr. Ragampeta Srinivas – Applications of Tandem Mass Spectrometry to Studies on some Non-natural Amino Acid Peptides and Differentiation of some Isomeric Organic Molecules

Mariappandada Vairamani – Guanine-quadruplex Formation studied by Mass Spectrometry

Shantanu Sengupta – Vitamin B 12 Deficiency: A Risk Factor for Cardiovascular Disease in India

Dr. Mahesh Kulkarni – Mass Spectrometry for Proteomics and Drug Discovery

Dr. Utpal Tatu – Mass Spectrometric Identification of a Novel Trans-splicing Event in Giardia lamblia Heat Shock Protein 90.

Practical Applications of Modern Tools in Organic Synthesis and Purifications II (PAMTOSP 2)

April 2-4, 2012

IISER Pune organized 3-day workshop during April 2-4, 2012 on Practical Applications of Modern Tools in Organic Synthesis and Purifications II (PAMTOSP 2) under the prime sponsorship of Royal Society of Chemistry, UK. This event was also cosponsored by various Indian and multi-national companies and was attended by participants from diverse range of backgrounds. The workshop was inaugurated by Dr. Sourav Pal, Director, NCL, Pune. Others present for the inauguration were: Dr. K.N. Ganesh, Director, IISER Pune, Mr. David Clark from

RSC, UK, Ms. Jayshree Mistry from GSK and Mr. Rajesh Parishwad from RSC, India. Among the 200 participants, students, academician and industry-based participants are the major. This 3-day event covered a historical overview of high throughput chemistry, use of reagents and scavengers in organic chemistry, solution phase methodology for parallel chemistry, use of solid phase in organic chemsitry, purifications technologies for high throughput chemistry, new developments and techniques in organic chemistry, practical demonstration workshops and computational tools for library design. Lectures and demonstrations were given by eminent persons from academia and industry from both India and abroad.

Mini-symposium on Spectroscopy and Dynamics

April 20, 2012

This mini-symposium organized by Dr. Aloke Das at IISER Pune on April 20, 2012 was part of annual activities of ISRAPS (Indian Society for the Radiation and Phytochemical Society), BARC, Mumbai. The meeting covered discussion on a broad range of spectroscopy including Femtosecond transient absorption, Terahertz, Resonance Raman, Femtosecond stimulated Raman, Fluorescence, Gas phase photodissociation dynamics in supersonic jet, Photoluminescence microscopy and simulation on dynamics of DNA intercalation. About 100 participants including students and faculty from TIFR, BARC, IIT Mumbai, University of Pune and IISER Pune were present for the meeting. We had total eight speakers from various institutes like IIT Mumbai, BARC, TIFR and IISER Pune. Prof. L.S. Shashidhara, IISER Pune presented opening remarks by briefly mentioning about scientific activities of IISER Pune. Dr. Tulsi Mukherjee, Director, Chemistry Division, BARC, inaugurated the symposium.

National Workshop on Polymer Solar Cells (NWPSC-2012)

April 21-22, 2012

A national workshop on polymer solar cells (NWPSC-2012) was organized with the support of Department of Science and Technology, Govt. of India. The workshop was coordinated by Prof. R.P. Singh and Dr. Shouvik Datta.

IISER Pune-University of Glasgow Bilateral Symposium on Structure and Dynamics

December 10-12, 2012

A joint symposium with the Universities of Glasgow and Strathclyde on Structure and Dynamics was held at IISER Pune during December 10-12, 2012 under the auspices of the UKIERI. Ten faculty members from the two universities visited IISER Pune to participate at the symposium. About 15 faculty members from IISER Pune presented their work. More than 50 research students presented posters in the meeting. Some of the speakers at this symposium were Prof. Krishna Ganesh, Prof. Klaas Wynne, Dr. Mrinalini Puranik, Dr. Goetz Bucher, Dr. Serena Korr, and Dr. M. Jayakannan.

International Meeting on Chemical Biology (IMCB-2013)

May 26-28, 2013

IMCB-2013 is an initiative by IISER Pune to foster interest amongst Indian scientific community in the emerging field of Chemical Biology. The conference was inaugurated by Prof. C.N.R. Rao. Leading and pioneering researchers from both academia and industry from around the world showcased the challenges and latest developments in the field of Chemical Biology. The sessions were nicely balanced with a wide range of topics covering biomolecular structure and function to therapeutics. There were 28 invited talks and several poster presentations. A special session was also arranged to commemorate the 60th anniversary of the discovery of the DNA double helix structure. The meeting was coordinated by Dr. Srinivas Hotha and Dr. Srivatsan.

DST FIST Committee Meeting

September 29, 2012

The Chemistry group of the Institute submitted an application for grant under the DST's FIST (Funds for Infrastructure in Science and Technology) program. As a part of the requirement, the members of the Committee visited the institute on September 29, 2012 to assess the available infrastructure and academic achievements. Subsequently, DST sanctioned ₹6.0 crores for equipping the labs with 600MHz NMR and other equipment. The process of application and defending the proposal was managed by Dr. Jayakannan and Dr. Srinivas Hotha under the guidance of Prof. Ganesh.

Satellite Meeting of the Frontiers in Chemistry and Biology of Oligosaccharides (FCBO-2014)

January 18-19, 2014

The topics covered were (a) approaches to understanding the structure, dynamics and function of oligosaccharides, (b) glycoconjugates and carbohydrate vaccines, (c) challenges in the synthesis of glycoconjugates and (d) biomolecular self-assemblies. There were 25 invited talks. Some of the speakers were: Alexei Demchenko,University of Missouri, St. Louis, USA; Amit Basu, Brown University, U.S.A., Joseph Barchi Jr. National Cancer Institute, Frederick, USA; Cristobel Lopez, Instituto de quimica Organica General, Juan de la Cierva 3, Madrid, Spain; Daniel Werz, Technische Universitaet Braunschweig, Germany; Hien Nguyen, University of Iowa, U.S.A.; B. Maria Pinto, Simon Fraser University, Vancouver, Canada; Mikael Bols, Kemisk Institut, Copenhagen, Denmark; Monica Palcic, Carlsberg Laboratory, Copenhagen, Denmark; Ole Hidsgaul, Carlsberg Laboratory, Denmark; George Oodoherty, Northeastern University, Boston, U.S.A.; Francesco Nicotra, University of Milano-Bicocca, Italy; Shang-Cheng Hung, Academia Sinica, Taipei, Taiwan; Todd Lowary, University of Alberta, Edmonton, Canada; Hermen Overkleeft, Leiden Institute of Chemistry, Leiden, Sweden; Aloysius Serianni, CNRS Research (HDR), France; and Anthony Serianni, University of Notre Dame, Indiana, U.S.A.. Speakers from India were: Chitra Mandal, IICB, Kolkata; Dilip Dhavale, University of Pune; Raghavendra Kikkeri, IISER Pune; Chepuri Ramana, NCL, Pune; Suvarn Kulkarni, IIT, Bombay; Srinivas Hotha, IISER Pune; B. Venkateswara Rao, IICT, Hyderabad; and Kana Sureshan, IISER, Thiruvananthapuram. Over 160 participants registered for this meeting which was organized by Dr. Srinivas Hotha.

National Workshop on Fluorescence and Raman Spectroscopic Techniques

December 15-19, 2014

Dr. Mrinalini Puranik and colleagues organized a national workshop on fluorescence and Raman spectroscopic techniques at IISER Pune in December 2014. This unique workshop provided hands-on training to students, post-doctoral researchers and young faculty in the state-of-the-art laser based spectroscopic techniques present at IISER Pune. Theoretical and experimental concepts in spectroscopy were taught by practicing research scientists from India and abroad along with IISER faculty. A novel concept implemented at IISER Pune was a round-table discussion session on each technique. These discussions were led by practicing researchers and were aimed at providing advice on problems faced by participants in various applications. Other highlights of the meeting were the teaching sessions on three different techniques of super-resolution spectroscopy and training in assembling cost-effective fluorescence and Raman instrumentation. Thirty five senior scientists taught and presented their research to over a hundred participants from all over the country.

Theoretical Chemistry Symposium

December 18-21, 2014

The fourteenth Theoretical Chemistry Symposium (TCS) was organized by CSIR- National Chemical Laboratory (CSIR-NCL), Pune and IISER Pune from December 18-21, 2014. IISER Pune organized all the talks of the symposium on December 20th. Held biennially, TCS is the largest platform for theoretical and computational chemistry research in India. The focus of this symposium is to converge a large number of researchers working in diverse areas involving quantum mechanics, statistical mechanics, computational sciences, algorithm development and encompassing numerous applications including chemical reaction mechanisms and pathways, material science and nanotechnology, polymer physics and chemistry, biological systems and bio-nano interfaces. The symposium was attended by 10 international speakers, 65 national speakers, 400 students and other faculty participants. Approximately, 300 posters were presented during the symposium.

Visitors

Distinguished Scientists who have visited IISER Pune

Prof. Jean-Marie Lehn
Université de Strasbourg, France
Nobel Laureate in Chemistry (1987)

Prof. George Whitesides
Harvard University, USA

Prof. Ei-ichi Negishi
Purdue University, USA
Nobel Laureate in Chemistry (2010)

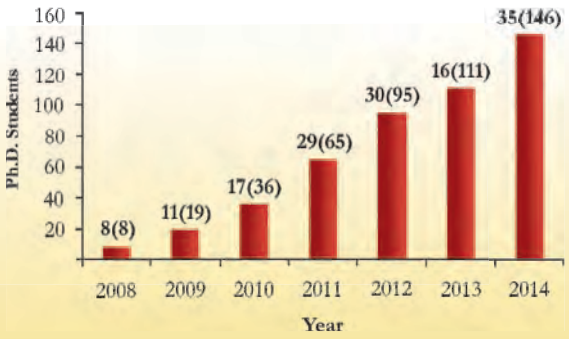
Prof. Venki Ramakrishnan
MRC Laboratory of Molecular Biology, UK
Nobel Laureate in Chemistry (2009)

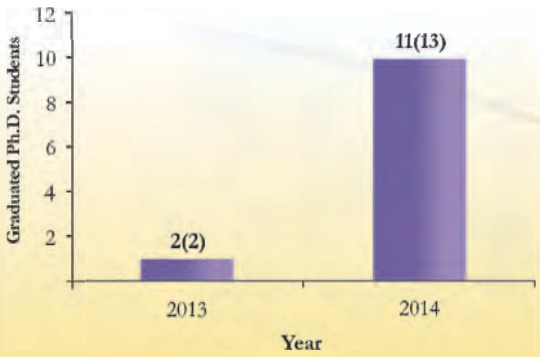
Prof. Jeremy Sanders
University of Cambridge, UK

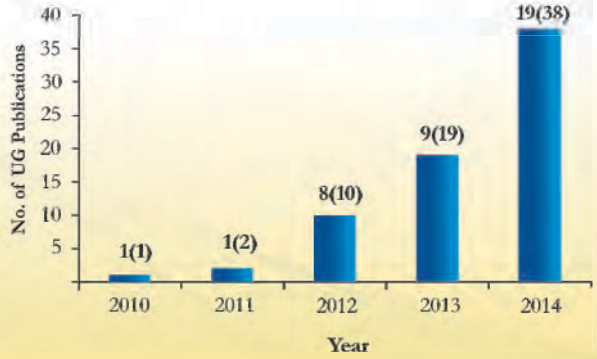
Prof. C. N. R. Rao
JNCASR, Bangalore, India

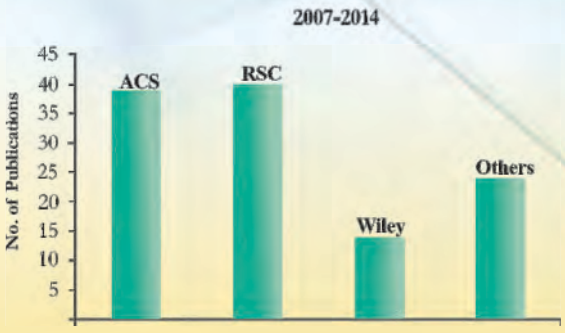
Department Statistics

Cumulative numbers in parentheses







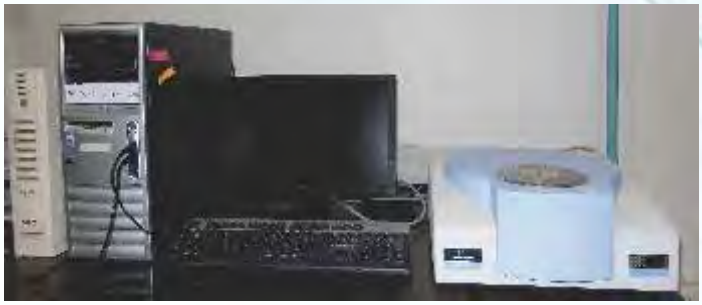


Instrument facilities in Chemistry

Name of Equipment	Year of Purchase	Details
Differential Scanning Calorimeter (DSC)	*2008*	TA
Thermogravimetric Analyzer (TGA)	*2008*	STA 6000, Perkin Elmer
Gel Permeation Chromatography (GPC)	*2008*	Viskotek Europe Ltd.
High Performance Liquid Chromatography-HPLC (6)	*2008-2011*	DIONEX, Waters, Agilent
Gas Chromatography - MS (GC-MS)	*2008*	GC-2010, Shimadzu
Gas Chromatography (GC)	*2013*	GC- 2014, Shimadzu
Liquid Chromatography - MS (LC-MS)	*2011*	Waters
High Resolution Mass spectrometer (HRMS)	*2011*	SYNAPT G2 HDMS Hybrid, Waters
Polarizing Light Microscope	*2008*	Leica DM2500P Microscope with DFC500 Camer
CHN Analyzer	*2010*	Vario EL cube, Elementar Analysensysteme GmbH
Gas adsorption Instrument	*2010*	Max Adsorption, aqua3 (BEL Japan Inc International Division)
UV-Vis Absorbance Spectrophotometer - 4 Nos	*2008-2010*	Chemito UV 2600 -4 nos, Evolution 300 - 01 nos, Varian Model Cary 300 Bio-2 nos, Lambda 45, Lambda 35, Shimadzu UV-VIS Spectrophotometer-3,
Steady State Fluorescence Spectrophotometer	*2011*	Flurolog - 3, Fluromax- 02 nos
Pico-second TCSPC Life time setup	*2008*	Assembled
Circular Dichroism (CD)	*2009*	J-815 CD Spectrometer, Jasco
FT-IR Spectrometer	*2008*	Nicolet 6700 FT-IR, Thermo
Isothermal Calorimeter (ITC)	*2008*	Itc200, Micro Cal
Cyclic Voltametry (CV)	*2008*	EPSILONE2
Dynamic Light Scattering (DLS)	*2009*	MALVERN
Automatic Solution Viscometer	*2008*	Schott - Instruments - GmbH

Name of Equipment	Year of Purchase	Details
Four Probe Conductivity Set-up	*2008*	PID-200 KETHLEY
Microwave-based Peptide Synthesizer	*2011*	CEM
DNA Synthesizer	*2010*	Applied Biosystems
Peptide Synthesizer	*2008*	Applied Biosystems
Cooling cabinet - 3 nos	*2010*	UNICHROMAT 1500 PRO
MALDI-TOF-TOF-MS	*2008*	4800 Plus, Applied Biosystems
Single crystal X-ray Instrument - Institute Facility	*2010*	Brucker
Wide Angel Powder X-ray diffraction Instrument	*2010*	Brucker
500 MHz Bucker NMR - Institute Facility (Central)	*2008*	Brucker
400 MHz JEOL NMR- Institute Facility (Central)	*2008*	Jeol
Automated Flash Chromatography system	*2014*	Yamazen
Steady state fluorescence spectrometer	*2014*	EDINBURH INSTRUMENTS FLS 980
High Performance Computing Cluster	*2014*	Hinditron Infosystems Pvt. Ltd.
600 MHz NMR Spectrometers	*2014*	Bruker
400 MHz NMR Spectrometers	*2014*	Bruker
Single Crystal X-Ray Diffractometer	*2014*	Bruker
Glove box & solvent purification system	*2014*	MBraun
Nano Drop 8000 Spectrophotometer	*2014*	Thermofischer
Femtosecond Fluorescence up conversion	-	Assembled
Gas Phase Spectroscopy	-	Assembled
Ultraviolet Resonance Raman Instrument	-	Assembled
Free Raman Imaging Microscope	-	Assembled

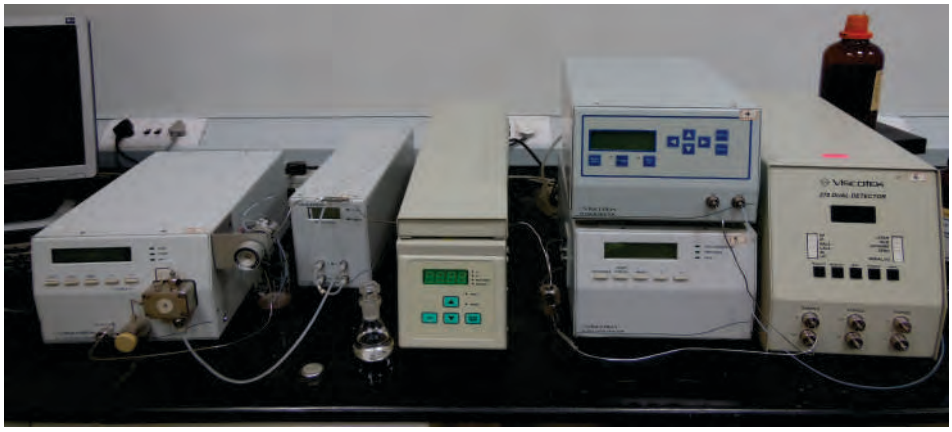
Differential Scanning Calorimeter (DSC)



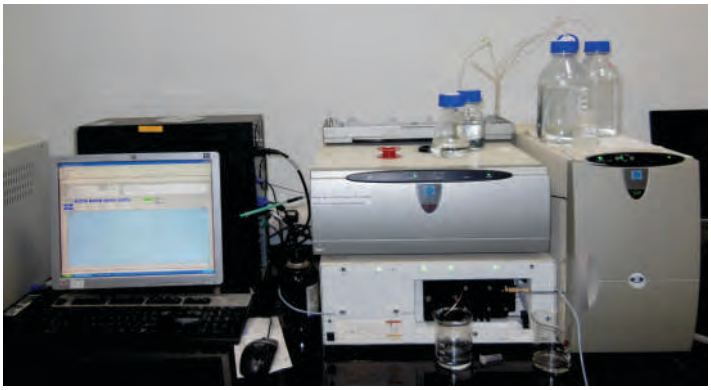
Thermogravimetric Analyzer (TGA)

Gas Chromatrography

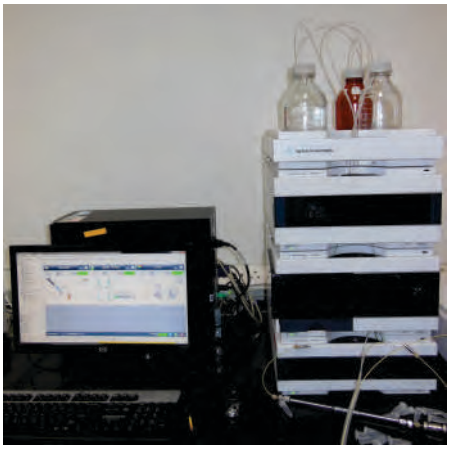
Gas Chromatrography-Mass Spectrometry (GC-MS)



Gel Permeation Chromatography (GPC)

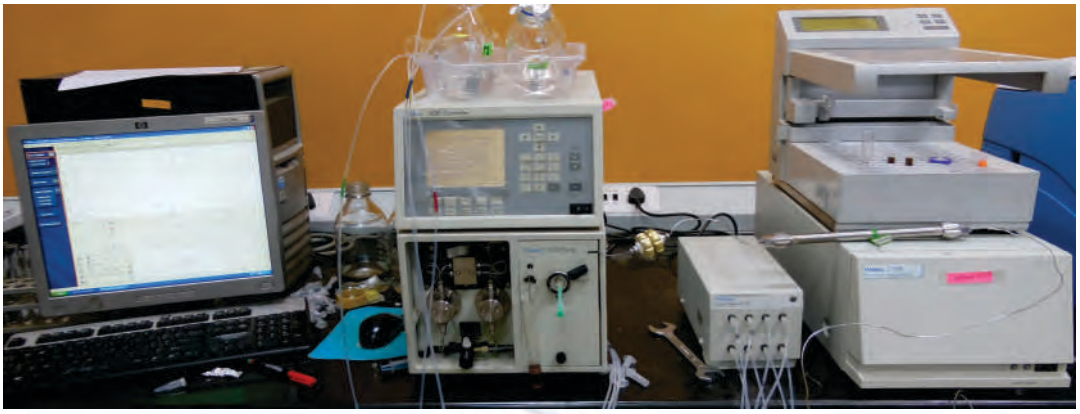


High Performance Liquid Chromatography- HPLC
Make – DIONEX

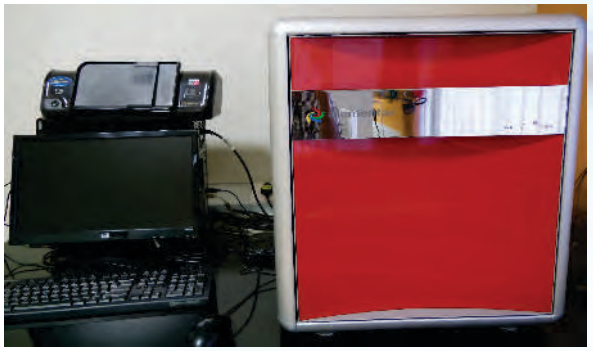


High Performance Liquid Chromatography HPLC
Make: Agilent

Polarizing Light Microscope
Make - Leica

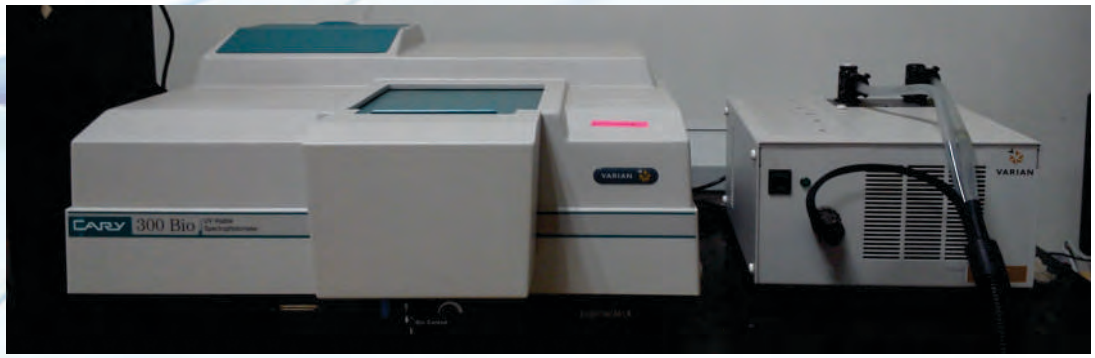


High Performance Liquid Chromatography- HPLC
Make: WATERS



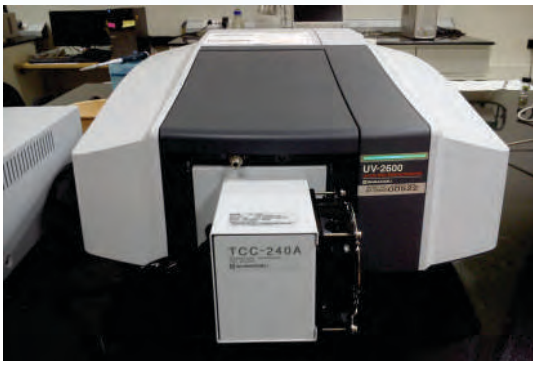
CHN Analyzer

Gas adsorption Instrument

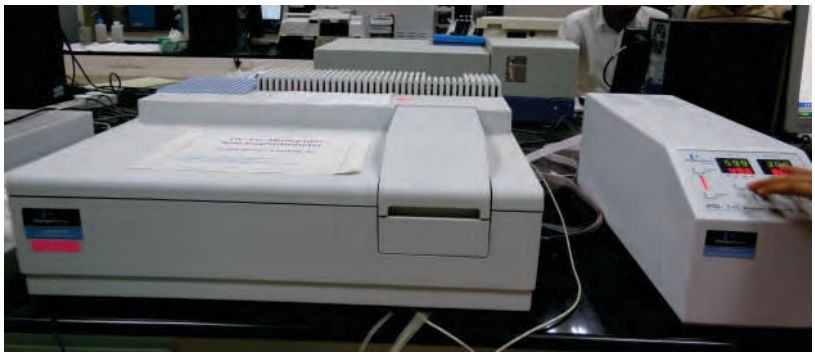


UV-Vis Absorbance Spectrophotometer Make – VARIAN

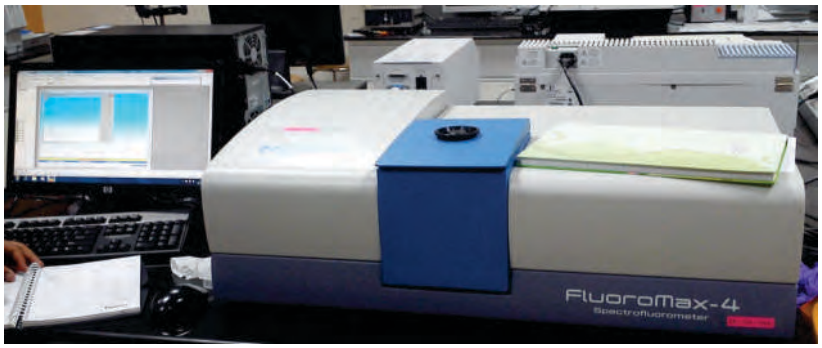
UV-Vis Absorbance Spectrophotometer Make – THERMO



UV-Vis Absorbance Spectrophotometer Make – SHIMADZU

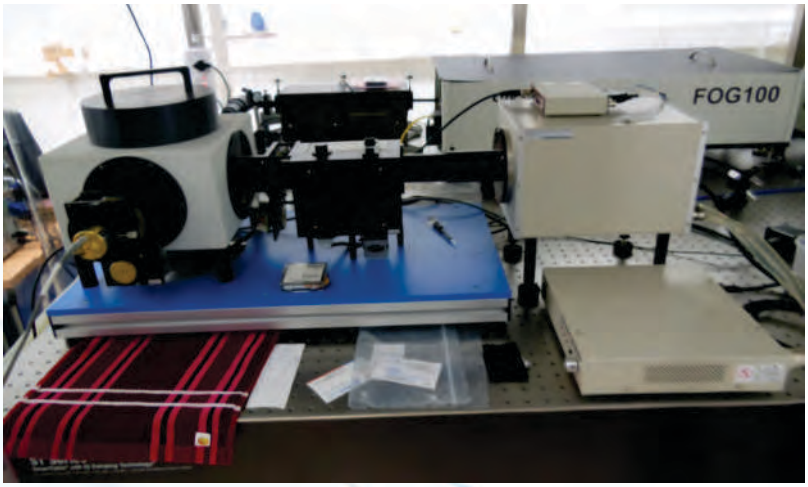


UV-Vis Absorbance Spectrophotometer Make – PERKIN ELMER



Fluorescence Spectrophotometer
Make: HORIBA
MODEL:Fluoromax-4

Fluorescence Spectrophotometer - Fluorolog
Make:HORIBA



Pico-second TCSPC
Life time setup

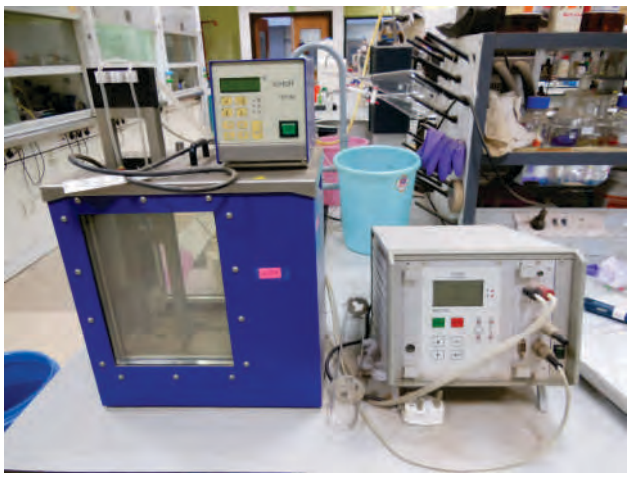
Circular Dichroism (CD)
Make- JASCO

FT-IR Spectrometer
Make- THERMO

Isothermal Calorimeter (ITC)
Make- MIRCOCAL ITC200

Cyclic Voltametry (CV)

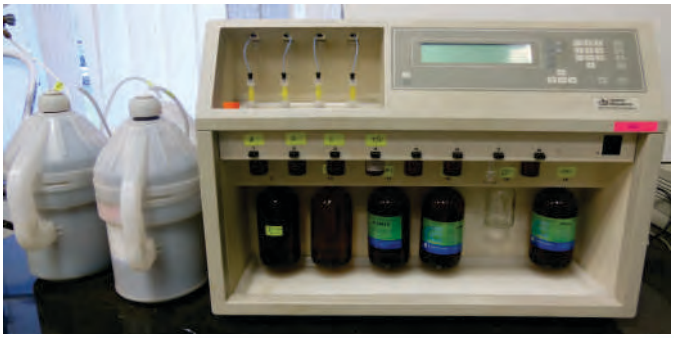
Dynamic Light Scattering (DLS)
Make: MALVERN



Automatic Solution Viscometer
Make: SCHOTT

Four Probe Conductivity Set-up
Make: KETHLEY

Microwave-based Peptide Synthesizer
Make:CEM



DNA Synthesizer
Make:APPLIEDBIOSYSTEMS

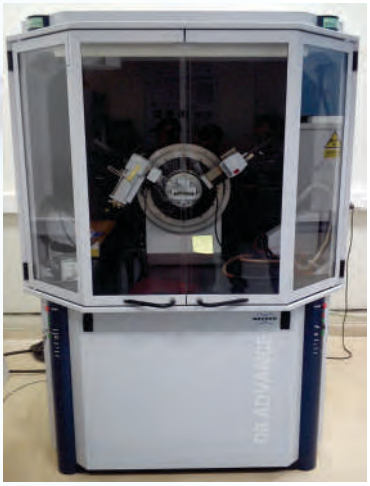
PEPTIDE SYNTHESIZER
Make:APPLIEDBIOSYSTEMS

COOLING CABINET
UNICHROMAT 1500 PRO

MALDI-TOF-TOF-MS
Make: APPLIEDBIOSYSTEMS

High Resolution
Mass spectrometer (HRMS)
Make - WATERS

Single crystal X-ray Instrument
Make - BRUKER



Wide Angel Powder
X-ray diffraction Instrument
Make: BRUKER

500 MHz
Bucker NMR

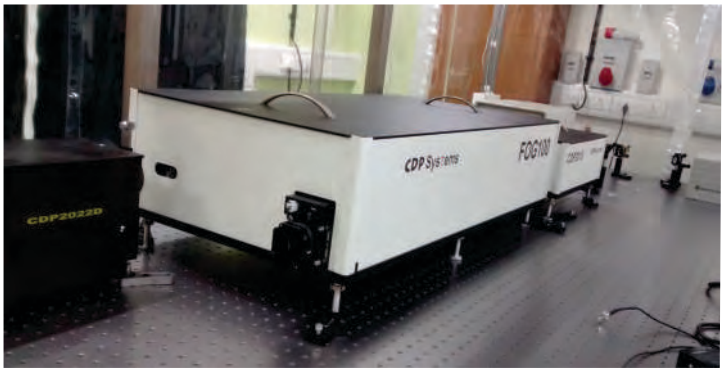
400 MHz
JEOL NMR

600 MHz
Brucker NMR

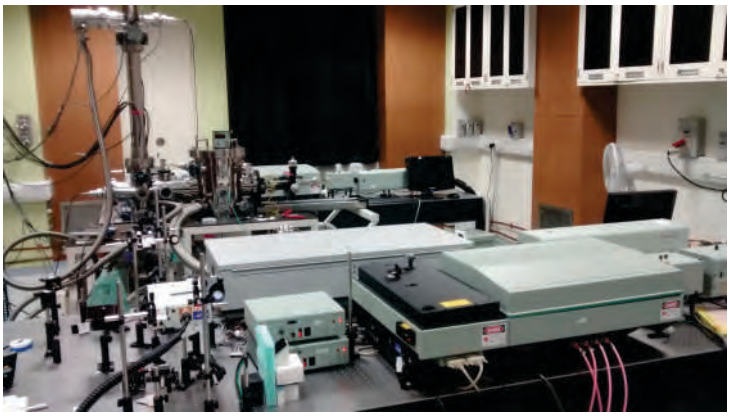
400 MHz
Brucker NMR

Glove Box & Solvent Purification System
Make- M BRAUN

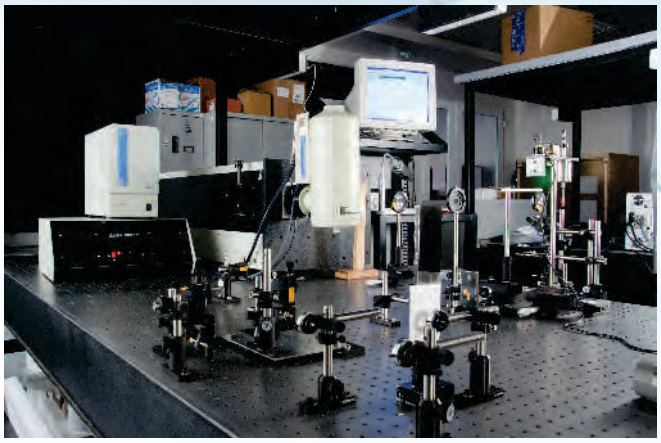
Terahertz Spectroscopy



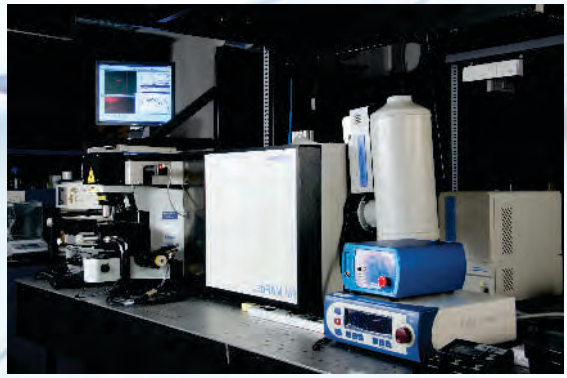
Femtosecond
Fluorescence Up Conversion



Gas Phase Laser Spectroscopy



Ultraviolet Resonance
Raman Instrument



Free Raman
Imaging Microscope

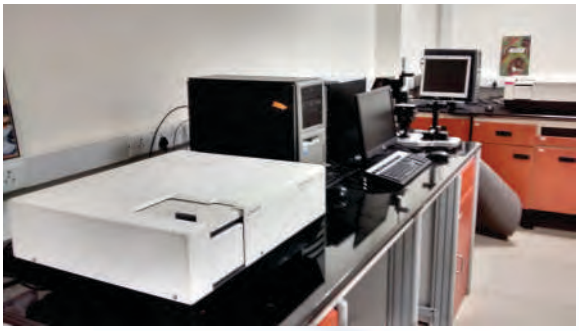
Steady State Fluoroscence Spectrometer
Make-EDINBURH
INSTRUMENTS FLS 980

Automated Flash Chromatography System
Make- YAMAZEN CORPORATION

Research Laboratory
In Main Building
Chemistry Wing

Research Laboratory
In Mendeleev

Research Laboratory
in Mendeleev



Instrumentation Facility for Undergraduate Students

Chemical Laboratory Facility for Undergraduate Students

Safety in Chemistry@IISER Pune

Environment, Health and Safety Committee, IISER Pune

IISER Pune Safety Committee (EHSC) works to fulfil its mission of safety and scope of its service. EHSC has good representation from academic departments and receives helpful administrative support.

Safety Goals: Reviewing Safety and Chemical Hygiene Plan (CHP); Conducting general and laboratory safety training, laboratory inspections and incident reporting; targeting specific safety issues identified during laboratory inspections; enhancing the awareness general and Lab Safety among IISER fraternity, evaluating undergraduate teaching lab safety, revival of Safety Manual.

Accomplishments:

Chemical Hygiene Plan (CHP): The EHSC continues to review and update safety-related policies, procedures and appendices. The primary goals of the program are to increase awareness, communication and safety team (Emergency Response Team) and to ultimately promote a culture of safety and trust at IISER Pune.

General Safety and Laboratory Safety Training

- EHSC, IISER-Pune as a regular practice conducts safety training for all students and staff by a professional authorized agency. IISER Pune conducts *Basic fire safety and Life Saving Skills* programme biannually. During the academic year beginning undergraduates (new batch) are exposed to training followed by PhD/project students/security staff and lab assistants.
- Institute has a safety manual for students' benefits and education for the safe practices.

Following very Important Hands on Skills are usually taught during the Programme:

Fire Fighting during Safety Training Programme

CPR (Cardio Pulmonary Resuscitation) on a Mannequin. Artificial Respiration, Chest Compressions, First Aid: Managing Wounds, Fractures, Bleeding, First Aid to Electrocution, Treating a Choking Victim, Fire Prevention and Fire Fighting, Chemistry and Classification of Fire, Practical use of Fire Extinguishers on Live Fire, LPG and Domestic Safety, Fighting Fire without Extinguishers, First Aid for Fire Burns and Life Saving Techniques. Safety presentations were also delivered to PhD students to teach the safe practices in laboratories across the divisions. Few images of Safety training are attached.

- EHSC focuses on procuring personal protective equipment (PPEs) for the undergraduate and research students every year.
  - IISER-Pune invested on quality lab coats and goggles. It is compulsory to wear personal protective equipment to avoid the health hazard in the laboratories.
  - First Aid box has been installed in each and every lab, Lecture Hall complex and also in few main receptions.
  - Fluorescent signage boards for the safety exits and for the safe guidelines have been installed in the labs and common areas.
  - Special Masks, stretchers, safety ladders have been procured
  - Based on the need safety fire extinguishers are procured and refilled
- Chemical Waste Management/ Disposal:
  - Students have been trained to segregate the chemical waste
  - Halogenated and non-halogenated solvent waste are collected in a separate containers
  - Silica gel, sand, Sodium sulphate, etc are collected as solid waste separately
  - Sharp items such as broken glassware, needles waste are segregated

IISER Pune has a contract with a government authorized agency to dispose the waste generation.

- Water Management: IISER Pune has built water purification plant for the drainage water waste.
- Inspection and Incident Reporting: As a common practice lab visits are done by the safety committee regularly. Safety visits are of two types one is routine safety visit and another one is a surprise visit. In the routine safety checks students are taken on a round to teach them about different kinds of safety measures and hazards due to ill plans.

❖ RSC-CRSI-IISER-NCL Safety Workshop, April 2014 held @ IISER Pune

Under the banner RSC (UK)–CRSI, India we arranged first of its kind one day Safety Workshop on "Safety in Chemical lab" for college and universities students and faculty. There were around 100 participants for this workshop. Director IISER Pune and Director, NCL inaugurated the workshop with initial remarks. Morning session had lectures on safety by experts in safety from RSC members, UK and experts from India. Afternoon, practical workshop was conducted in few groups.

EHS Committee

Dr. Ramakrishna G. Bhat (Chairperson)
Dr. Sunil Nair (Member)
Dr. Partha Hazra (Member)
Dr. Girish Ratnaparkhi (Member)
Dr. Y. Rajput (Member)
Dr. Shabana Khan (Member)

Lab Safety Rules

POLICIES

- Ensure safe handling of chemicals by referring to Material Safety Data Sheet (MSDS) or ask the supervisor
- Before carrying out the reaction (experiment) or use of any instruments ask the supervisor for the assistance.
- Know the location of the (i) **"Emergency Shut-Off"** switches in the lab and instrument room (ii) **Emergency Exits** and (iii) **fire extinguishers.**
- Report "All" accidents, no matter how minor, to the Supervisor/Safety In-Charge immediately
- Do not work alone in the laboratory.
- Student with medical/Health concerns should seek the advice of a Doctor before attending labs.

RULES

- **Wear approved safety goggles and lab coat at all the times.** If you have spilled chemical in your eyes, flush with water in an eye wash station for 10 to 15 minutes. Use safety shower in case of chemical spillage on body. Notify the incident to Supervisor and Safety In-Charge.
- **Confine long hair** whenever working in the laboratory.
- **Wear Shoes while working in the lab.** Feet must be adequately covered. Open toed shoes or sandals are not permitted in the laboratory.
- **Keep benches free from clutter.** Backpacks, coats and personal items must be put away.
- **NO eating or drinking in the laboratory.**
- **NO tobacco products in the laboratory. NO Smoking in the Campus premises.**
- **Familiarize yourself with the lab** (equipment, chemicals).
- **Never mouth a pipette, use a rubber bulb.**
- **Never leave an experiment unattended,** particularly those require heat or running water.
- **Report all spills especially mercury spill** to Supervisor and Safety in Charge.
- **Do not use broken or chipped glassware** and dispose them in the glass disposal box.
- **Segregate the waste solvents** appropriately for the proper disposal.
- **Used syringe needles should be dropped in syringe disposal box,** and do not dump waste paper in the broken glass/needle disposal boxes.
- **Use glycerin when inserting glass tubing or thermometers into rubber stoppers.**
- **Do not perform unauthorized experiments in the lab.**
- **Do not use torn out electric wired equipment.**
- **Follow the special instructions** to use X-ray, Lasers, and radioactive materials, electrical hazard etc. (Contact Supervisor/Expert's Advice needed)
- **Follow special instructions and, be careful while handling and disposing Biohazardous samples** (Contact, Safety In-Charge, Biology Division)
- If you are **allergic to any chemicals/Solvents** please give the details to supervisor.

Main Building, IISER Pune

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Website : www.iiserpune.ac.in