IISER PUNE - TEMPLE UNIVERSITY
SUMMER PROGRAM 2018

IISER PUNE

RESEARCH PROJECTS IN CHEMISTRY

May-July, 2018

ABOUT THE PROGRAM

Temple University and IISER Pune have signed a Memorandum of Understanding focusing on student and faculty exchange with emphasis on joint research programs. To strengthen this initiative, internships have been initiated for students from Temple University to work in research groups at IISER Pune.

This brochure includes information on the faculty and research projects that are open to accept students for Summer 2018 as part of this Program.

Applications: Interested students should directly contact the Project Investigator of interest. The initial inquiry should include a resume/CV, a transcript and a statement describing prior research experience, career goals and why the particular project is of interest.

Visa and Travel: Students will be responsible for obtaining **research visa** for participation in the summer research program. Students are responsible for travel arrangements. The most convenient would be to fly to Pune International Airport (PNQ) which has some international connections or fly to Mumbai (BOM) airport. IISER Pune is 3 hour drive from Mumbai airport .

Housing and Food: On-campus housing will be provided with access to several cafeteria. The estimated cost of housing and food: USD 300 per month.

For any questions related to visa, travel, housing and food, please contact Dr. Naresh Sharma (International Relations). Email: naresh.sharma@iiserpune.ac.in

General information: Inquiries about the program should be directed to arun@iiserpune.ac.in

JANUS PEPTIDE NUCLEIC ACIDS (PNA) AS PROGRAMMABLE SELF ASSEMBLING SYSTEMS

Project Investigator: Professor K. N. Ganesh, (Director at IISER Tirupati, and Professor at IISER Pune)

Preferred scientific requirements: Course in synthetic organic chemistry/bio-organic chemistry/hands on experience in synthetic chemistry preferred.

Research summary: Peptide Nucleic Acids are excellent mimics of DNA/RNA and bind strongly to cDNA/RNA. It is proposed to make bifacial (Janus) PNAs that can recognize complementary DNA/RNA/PNA to form mixed duplexes and that can simultaneously recognise two DNA/RNA targets. These self assemble in a programmable way to lead to two dimensional PNA/DNA/RNA scaffolds that will have interesting material properties.

Representative Publications

1. D. R. Jain, L. Anandi, M. Lahiri, and K. N. Ganesh, Influence of Pendant Chiral C#-(alkylideneamino/guanidino) Cationic Sidechains of PNA Backbone on Hybridization with Complementary DNA/RNA and Cell Permeability. J. Org. Chem. 2014, 79, 9567-9577.
2. D. R. Jain and K. N. Ganesh, Clickable Cγ-Azido(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.
3. S. Ellipilli and K. N. Ganesh, Fluorous Peptide Nucleic Acids: PNA Analogues with Fluorine in Backbone (γ-CF2-apg-PNA) Enhance Cellular Uptake. J. Org. Chem. 2015, 80, 9185-9191.
4. S. Ellipilli, R. V. Murthy and K. N. Ganesh, Perfluoroalkylchain conjugation as a new tactic for enhancing cell permeability of peptide nucleic acids (PNAs) via reducing the nanoparticle size. Chem Commun, 2016, 52, 521-524.

Contact Info: E-mail: kn.ganesh@iiserpune.ac.in, Tel: +91-20-2590-8021
Group Web Page: http://www.iiserpune.ac.in/~kn.ganesh
Project Location: Student may either work at IISER Pune or at IISER Tirupati

BIOMEDICALLY SIGNIFICANT GIANT GLYCOCONJUGATES SYNTHESES BY GOLD-CATALYZED GLYCOSIDATIONS

Project Investigator: Prof. Srinivas Hotha

Preferred scientific requirements: Organic Synthesis, Basic knowledge of carbohydrate chemistry.

Research summary: Glycosylation is an important post-translational modification and many glycoconjugates are established to be important for many signal-transduction processes at cellular level. Many oligosaccharides are currently sold as prebiotic and probiotic foods and several glycoconjugates are in different stages of drug discovery enterprise. Over the last one decade, we discovered and pioneered gold-catalysed glycosidation methods for the synthesis of oligosaccharides. Method developed in the group is robust, versatile and applicable to a wide range of glycosides. All major carbohydrate epitopes present in the glycocalyx of Mycobacterium tuberculosis are synthesized in the group. Giant oligosaccharide syntheses deploying methods developed in the group is the main focus of the laboratory. Efforts are also in place to utilize those glycans for developing diagnostics and conjugate candidate vaccines for infectious diseases.

Representative Publications

1. S. A. Thadke, B. Mishra, M. Islam, S. Pasari, S. Manmode, B. V. Rao, M. Neralkar, G. O. Shinde, G. Walke, S. Hotha, [Au]/[Ag]-catalysed expedient synthesis of branched heneicosafuranosyl arabinogalactan motif of Mycobacterium tuberculosis cell wall, Nature Commun. 8, 14019 (2017).
2. M. Islam, G. P. Shinde, S. Hotha, Expedient synthesis of heneicosasaccharyl mannose capped arabinomannan of the Mycobacterium tuberculosis cellular envelope by glycosyl carbonate donors, Chem. Sci., 8, 2033-2038 (2017).
3. S. Pasari, S. Manmode, G. Walke, A versatile synthesis of pentacosafuranoside subunit reminiscent of mycobacterial arabinogalactan employing one strategic glycosidation protocol, Chem. Eur. J. 33, DOI:10.1002/chem.201704009 (2017)
4. B. Mishra, M. Neralkar, S. Hotha, Stable alkynyl glycosyl carbonates: Catalytic anomeric activation and synthesis of a tridecasaccharide reminiscent of Mycobacterium tuberculosis cell wall lipoarabinomannan, Angew. Chem. Int. Ed. Eng. 55, 7786-7791 (2016).
5. S. A. Thadke, B. Mishra, S. Hotha, Facile synthesis of β- and α-arabinofuranosides and application to cell wall motifs of M. tuberculosis, Org. Lett., 15, 2566-2569 (2013)
6. S. A. Thadke, B. Mishra, S. Hotha, Gold(III)-catalyzed glycosidations for 1,2-trans and 1,2-cis furanosides, J. Org. Chem. 79, 7358-7371 (2014)

Contact Info: E-mail: s.hotha@iiserpune.ac.in, Tel: +91-20- 2590-8015
Group Web Page: http://www.iiserpune.ac.in/~s.hotha

DIRECT ORGANOCATALYTIC MULTICOMPONENT SYNTHESIS FOR THE CONSTRUCTION OF ENANTIOPURE BIOACTIVE COMPOUNDS

Project Investigator: Dr. Ramakrishna G. Bhat

Preferred scientific requirements: Preliminary knowledge in Organic chemistry or Research experience in synthetic organic chemistry and relevant laboratory techniques are preferred.

Research summary: Our Laboratory is involved in conducting the research in the field of Organic synthesis with a focus on organocatalysis and C-H functionalization. We aim our research with an emphasis on the development of new synthetic methods that facilitate the construction of complex and bioactive molecules. In this project, we will focus on the quinine/Cinhona thiourea derived catalysts for the effective organocatalysis for the novel C-C bond formation. The methodology is expected to provide the mechanistic insights and further lead to applications in the synthesis of enantiopure bioactive molecules and pharmaceuticals.

Representative Publications

1. Khopade T. M. Sonawane, A. D. Arora, J. S and Bhat, R. G. Direct Organocatalytic Multicomponent Synthesis of Enantiopure g-Butyrolactones via Tandem Knoevenagel-Michael-Lactonization Sequence Adv. Synth. Catal. 2017, 359, 1-7.
2. 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)
3. 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
4. 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)

Contact Info: E-mail: rgb@iiserpune.ac.in, Tel: +91-20- 2590-8092
Group Web Page: http://www.iiserpune.ac.in/~rgb

EXPLORING PEPTIDE FOLDAMERS TO DESIGN FUNCTIONAL BIOMATERIALS

Project Investigator: Dr. H. N. Gopi

Preferred scientific requirements: Synthetic organic chemistry background and knowledge or research experience in area of peptides and foldamers are preferred.

Research summary: Designing synthetic protein structures using non-natural amino acids has immense importance from the perspective of medicinal chemistry. In addition, these peptide foldamers also provided an excellent opportunity to design functional biomaterials. In this project, we would like to explore the utility of peptide foldamers composed of γ-amino acids towards the design of functional biomaterials such as nanotubes, microtubes, vesicles and gels. Recently, we demonstrated the casting of silver nanowires from foldamer nanotubes, mild temperature triggered controlled release of encapsulated molecules from the liposome-coiled- coil nano-composites containing γ-amino acids mutated coiled-coils, and utilization of γ-peptide hydrogels in the 2D cell cultures.

Representative Publications

1. Misra, R.; Sharma, A.; Shiras, A.; Gopi, H. N. Backbone Engineered γ-Peptide Amphitropic Gels for Immobilization of Semiconductor Quantum Dots and 2D Cell Culture. Langmuir 2017, 33, 7762.
2. Misra, R.; Reja, R. M.; Narendra, L. V.; George, G.; Raghothama, S.; Gopi, H. N. Exploring Structural Features of Folded Peptide Architectures in the Construction of Nanomaterials. Chem. Commun. 2016, 52, 9597.
3. Reja, R. M.; Khan, M.; Singh, S. K.; Misra, R.; Shiras, A.; Gopi. H. N. pH Sensitive Coiled Coils: A Strategy for Enhanced Liposomal Drug delivery. Nanoscale, 2016, 8, 5319.
4. Jadhav, S. V.; Misra, R.; Gopi, H. N. Foldamers to Nanotubes: Influence of Amino acid Side-chains in the Hierarchical Assembly of α, γ4 -Hybrid Peptide Helices. Chem. Eur. - J. 2014, 20, 16523.
5. 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.

Contact Info: E-mail: hn.gopi@iiserpune.ac.in, Tel: +91-20- 2590-8075
Group Web Page: http://www.iiserpune.ac.in/~hn.gopi/

REDOX GUIDED ANTIBIOTIC DISCOVERY

Project Investigator: Dr. Harinath Chakrapani

Preferred scientific requirements: Basic synthetic organic chemistry and compound characterization techniques.

Research summary: Perturbation of redox homeostasis is a component of mechanism of bactericidal antibiotics against infectious pathogens. Interrogating the redox proteome presents opportunities for new drug discovery, especially against drug-resistant pathogens. In this project, we propose to use small molecule tools to interrogate the thiol proteome to identify new targets for both gram-positive as well as gram-negative pathogens. This study will lay the foundation for new drug discovery with possibly unique mechanisms.

Representative Publications

1. Shukla, P.; Khodade, V. S.; Sharath Chandra, M.; Chauhan, P.; Mishra, S.; Siddaramappa, S.; Bulagonda, E. P.; Singh, A.; Chakrapani, H. "& "On Demand"; Redox Buffering by H2S Contributes to Antibiotic Resistance Revealed by a Bacteria-Specific H2S Donor"; Chemical Science 2017, 8, 4967-4972.
2. 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 Medicinal Chemistry Letters 2014, 5, 777-781.
3. Sankar, R. K; Kumbhare, R. S.; Dharmaraja, A. T.; Chakrapani, H. “A Phenacrylate Scaffold for Tunable Thiol Activation and Release” Chemical Communications, 2014, 50, 15323-15326.
4. 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” Journal of Medicinal Chemistry, 2012, 55, 553-557

Contact Info: E-mail: harinath@iiserpune.ac.in, Tel: +91-20- 2590-8090
Group Web Page: http://www.iiserpune.ac.in/~harinath/

PROBING NON-CANONICAL NUCLEIC ACID STRUCTURES IN CELLULAR ENVIRONMENT USING NUCLEOSIDE PROBES

Project Investigator: Dr. Seergazhi G. Srivatsan

Preferred scientific requirements: Courses or preferable research experience in organic synthesis and basic molecular biology techniques.

Research summary: Our group is interested in developing multifunctional nucleoside analogs, which could serve as common probes for analyzing nucleic acids simultaneously by fluorescence, NMR and X-ray crystallography techniques. The present project would involve the incorporation of such biophysical tools into therapeutically relevant oligonucleotide sequences and study their structure and recognition properties in real-time and in cellular environment by using a combination of fluorescence and NMR techniques.

Representative Publications

1. Tanpure, A. A.; Srivatsan, S. G. Conformation-sensitive nucleoside analogues as topology-specific fluorescence turn-on probes for DNA and RNA G-quadruplexes. Nucleic Acids Res. 2015, 43, e149.
2. 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.
3. Nuthanakanti, A.; Boerneke, M. A.; Hermann, T.; Srivatsan, S. G. Structure of the ribosomal decoding site RNA containing a Se-modified responsive fluorescent ribonucleoside probe. Angew. Chem. Int. Ed. 2017, 56, 2640–2644.
4. Manna, S.; Panse, C. H.; Sontakke, V. A.; Sangamesh, S.; Srivatsan, S. G. Probing human telomeric DNA and RNA topology and ligand binding in a cellular model by using responsive fluorescent nucleoside probes. ChemBioChem 2017, 18, 1604–1615.

Contact Info: E-mail: srivatsan@iiserpune.ac.in, Tel: +91-20-2590-8086

Group Web Page: http://www.iiserpune.ac.in/~srivatsan/

METAL ORGANIC FRAMEWORK (MOF) AND POROUS ORGANIC FRAMEWORKS (POF) FOR CHARGE STORAGE AND ELECTROCHEMICAL APPLICATIONS

Project Investigator: Dr. R. Vaidhyanathan

Preferred scientific requirements: Knowledge and experience in basic chemistry, electrochemistry and in materials chemistry would be helpful. Also, some experimental research experience in physical chemistry or materials characterization is plus.

Research summary:

Project 1: The work involves the investigation of the charge storage capacities of some of the MOFs and POFs synthesized in our lab. Another task would be to investigate new redox active nano materials for their potential in water-splitting. Student would be going through the synthesis and then along with some PhD students would be carrying out the electrochemical studies (reversible Li ion storage, Supercapacitor, three-electrode electrochemical measurements for water splitting analysis). We would be having detailed group discussions on this topic during the entire summer which could be extremely beneficial. We have plans to arrange short visits to couple of electrochemical companies and also to advanced electrochemical characterization centers.
Project 2: Developing advanced Metal Organic Frameworks for gas separation applications. Student would be developing (design and synthesis) metal organic frameworks most suited for CO2 capture and methane storage. Would be carrying out complete material characterization and a range of adsorption studies with the help of PhD students.

Representative Publications

1. S. Nandi, S. K. Singh, D. Mullangi, R. Illathvalappil, L. George, C. P. Vinod, S. Kurungot, and R. Vaidhyanathan. Low Band Gap Benzimidazole COF Supported Ni3N as Highly Active OER Catalyst. Adv. Energy Mater., 2016, 1601189.
2. D. Mullangi, V. Dhavale, S. Shalini, S. Nandi, S.Collins, T. Woo, S. Kurungot, and R. Vaidhyanathan. Low-Overpotential Electrocatalytic Water Splitting with Noble-Metal-Free Nanoparticles Supported in a sp3N-Rich Flexible COF. Adv. Energy Mater., 2016, 6, 1600110.
3. S. Nandi, P. D. Luna, T. D. Daff, J. Rother, M. Liu, W. Buchanan, A. I. Hawari, T. K. Woo, R. Vaidhyanathan. A single-ligand ultra-microporous MOF for precombustion CO2 capture and hydrogen purification. Sci., Adv., 2015, 1, e1500421.
4. S. Nandi, S. Collins, D. Chakraborty, D. Banerjee, P. K. Thallapally, T. K. Woo, and R. Vaidhyanathan, Ultralow Parasitic Energy for Postcombustion CO2 Capture Realized in a Nickel Isonicotinate Metal–Organic Framework with Excellent Moisture Stability. J. Am. Chem. Soc. 2017, 139, 1734–1737.

Contact Info: E-mail: vaidhya@iiserpune.ac.in, Tel: +91-20-2590-8073
Group Web Page: http://www.iiserpune.ac.in/~vaidhya

DESIGN, SYNTHESIS AND CHARACTERIZATION OF MOLECULAR FERROELECTRIC MATERIALS

Project Investigator: Dr. Ramamoorthy Boomishankar

Preferred scientific requirements: Courses: Main Group and transition metal Chemistry and preferably Solid-state chemistry. Research experience in synthetic inorganic or organic chemistry laboratory.

Research summary:

Ferroelectrics are special class of dielectrics having switchable spontaneous electric polarization that can be reversed or reoriented by application of an external electric field. Materials havin ferroelectric, multiferroic and magnetoelectric properties are of major research interest due to their application in high-technique devices. Traditionally, ceramic materials of perovskite family are used as commercial ferroelectrics. In this effort, a range of new age materials viz., polymers, organic-inorganic hybrids and small molecules have been explored to overcome certain limitations associated with ceramic materials. Our group has been interested in utilizing various P-N scaffolds to generate polar ordered materials with potential ferroelectric properties. Thus, pyridyl functionalized di- and tripodal phosphoramide ligands have been employed to specifically obtain metal-organic assemblies in discrete (cages and cavitands) structures, 1D-helical and 2D-layered networks in polar point groups. Polarization in these materials was found to originate from the choice of anions, dimensionality of the frameworks and guest molecules present in them. In addition, we have also been interesting in examining polar phosphorus containing organic and organic-inorganic hybrid salts as ferroelectric materials.

Representative Publications

1. A. K. Srivastava, B. Praveenkumar, I. K. Mahawar, P. Divya, S. Shalini and R. Boomishankar Anion Driven [Cu II L 2] n Frameworks: Crystal Structures, Guest-Encapsulation, Dielectric, and Possible Ferroelectric Properties, Chem. Mater, 26, 3811 (2014).
2. A. K. Srivastava, P. Divya, B. Praveenkumar and R. Boomishankar, Potentially Ferroelectric [Cu II L 2] n Based Two-Dimensional Framework Exhibiting High Polarization and Guest-Assisted Dielectric Anomaly, Chem. Mater, 27, 5222 (2015).
3. A. K. Srivastava, T. Vijayakanth, P. Divya, B. Praveenkumar, A. Steiner and R. Boomishankar, Altering polarization attributes in ferroelectric metallo-cavitands by varying hydrated alkali-metal guest cations, J. Mater. Chem. C, 5, 7352 (2017).
4. A. Yadav, A. K. Srivastava, P. Kulkarni, P. Divya, A. Steiner, B. Praveenkumar and R. Boomishankar, Anion-induced ferroelectric polarization in a luminescent metal organic cage compound, J. Mater. Chem. C, 5, 10624 (2017).

Contact Info: E-mail: boomi@iiserpune.ac.in, Tel: +91-20- 2590-8208
Group Web Page: http://www.iiserpune.ac.in/~boomi/

PHOTOPHYSICS OF METAL ION DOPED CESIUM LEAD HALIDE PEROVSKITE NANOCRYSTALS

Project Investigator: Dr. Angshuman Nag

Preferred scientific requirements: Course in spectroscopy, solid state chemistry and interest for colloidal synthesis of nanocrystals.

Research summary: Colloidal cesium lead halide perovskite Nanocrystals have been recently established as a new kind of defect-tolerant material, exhibiting interesting optoelectronic properties. Presently, we are doping various metal ions such Mn^{2+} and Bi^{3+} in such nanocrystals, for tailoring electronic and optical properties. Broadly, the summer student is expected to synthesize such doped nanocrystals following protocols existing in our laboratory, and then study the effect of doping on luminescence (both steady-state and time resolved) and other optical properties.

Representative Publications

1. Pradhan, N.; Adhikari, S. D.; Nag, A.; Sarma D. D. Luminescence, Plasmonic and Magnetic Properties of Doped Semiconductor Nanocrystals: Current Developments and Future Prospects. Angew. Chem. Int. Ed. 2017, DOI: 10.1002/ange.201611526.
2. Mir, W. J.; Jagadeeswarara, M.; Das, S.; Nag, A. Colloidal Mn-Doped Cesium Lead Halide Perovskite Nanoplatelets. ACS Energy Lett., 2017, 2, 537–543.
3. Yettapu, G. R.; Talukdar, D.; Sarkar, S.; Swarnkar, A.; Nag, A.; Ghosh, P.; Mandal, P. Thz Conductivity within Colloidal CsPbBr3 Perovskite Nanocrystals: Remarkably High Carrier Mobilities and Large Diffusion Lengths. Nano Lett. 2016, 16, 4838.
4. Tandon, B.; Yadav, A.; Nag, A. Delocalized Electrons Mediated Magnetic Coupling in Mn-Sn codoped In_2O_3 Nanocrystals: Plasmonics shows the way. Chem. Mater. 2016, 28, 3620.
5. Swarnkar, A.; Chulliyil, R.; Ravi, V. K.; Irfanullah, M.; Chowdhury, A.; Nag, A. Colloidal CsPbBr3 Perovskite Nanocrystals: Luminescence beyond Traditional Quantum Dots. Angew. Chem. Int. Ed. 2015, 54, 15424.

Contact Info: E-mail: angshuman@iiserpune.ac.in, Tel: +91-20-2590-8117

Group Web Page: http://www.iiserpune.ac.in/~angshuman/

EXPLORING N→Π* NON-COVALENT INTERACTION IN PEPTIDES USING GAS PHASE LASER SPECTROSCOPY AND QUANTUM CHEMISTRY CALCULATIONS

Project Investigator: Dr. Aloke Das

Preferred scientific requirements: Spectroscopy course and/or Research experience in Laser spectroscopy.

Research summary: n→π* non-covalent interaction is widely present in biomolecules (proteins, nucleic acids, neurotransmitters etc.) as well as materials. In spite of its immense significance in the structures of various molecular systems, this non-covalent interaction has been recognized only recently (during last two decades) by the scientific community due to its counterintuitive and weak (strength) nature. In this project, we will explore this weak interaction in dipeptides/tripeptides using UV/IR laser based various gas phase spectroscopic techniques combined with quantum chemistry calculations. In-depth understanding of this weak interaction might help in designing better functional materials and drugs.

Representative Publications

1. Santosh Kumar Singh, Jamuna K. Vaishnav and Aloke Das*, Experimental observation of structures with subtle balance between strong hydrogen bond and weak n→ π* interaction: Gas phase laser spectroscopy of 7-azaindole⋯ fluorosubstituted pyridines, J. Chem. Phys., 145, 104302 (2016).
2. Santosh Kumar Singh, Kamal Kumar Mishra, Neha Sharma, and Aloke Das * , Direct spectroscopic evidence for an n → π* interaction, Angew. Chem. Int. Ed., 128, 7932 (2016).
3. Santosh Kumar Singh * and Aloke Das *, n→π* interaction: A rapidly emerging non-covalent interaction, Phys. Chem. Chem. Phys. 17, 9596 (2015). (Invited Perspective)
4. Santosh Kumar Singh, Sumit Kumar and Aloke Das *, 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. 16, 8819 (2014). (Appeared as front inside coverpage)

Contact Info: E-mail: a.das@iiserpune.ac.in, Tel: +91-20- 2590-8078
Group Web Page: http://www.iiserpune.ac.in/~a.das/

MOLECULAR DYNAMICS SIMULATION OF STRUCTURE AND DYNAMICS OF POLYMER ELECTROLYTE MEMBRANES

Project Investigator: Dr. Arun Venkatnathan

Preferred scientific requirements: Course or research experience in application of Molecular Dynamics simulations and/or computer programming experience are preferred.

Research summary: Perfluorosulfonic Acid and Polybenzimidazole are polymeric materials which can serve as potential fuel cell electrolytes. In this project we propose an examination of structure and dynamics of these membranes with humidification or other charge carrier solvents (ionic liquids) using classical Molecular Dynamics simulations. The molecular level insight from simulations is expected to enhance an understanding of structure and molecular transport and can lead to the development of efficient membrane materials for fuel cell applications.

Representative Publications

1. S. Sengupta, R. Pant, P. Komarov, A. Venkatnathan and A. V. Lyulin, Atomistic simulation study of the hydrated structure and transport dynamics of a novel multi acid side
chain polyelectrolyte membrane, Int. J. Hydrogen Energy, 42, 27254 (2017).
2. R. Pant, M. Kumar and A. Venkatnathan, Quantum Mechanical Investigation of Proton Transport in Imidazolium Methanesulfonate Ionic liquid , J. Phys. Chem. C, 121, 7069 (2017).
3. M. More, A. P. Sunda, and A. Venkatnathan, Polymer chain length, phosphoric acid doping and temperature dependence on structure and dynamics of ABPBI [poly(2,5-benzimidazole)] polymer electrolyte membrane, RSC Advances, 4, 19746 (2014).
4. A. P. Sunda and A. Venkatnathan, Molecular Dynamics Simulations of Side Chain Pendant of Perfluorosulfonic Acid Polymer Electrolyte Membranes, J. Mater. Chem. A.,1, 557 (2013).

Contact Info: E-mail: arun@iiserpune.ac.in, Tel: +91-20-2590-8085

Group Web Page: http://www.iiserpune.ac.in/~arun/


IISER PUNE
...where tomorrow's science begins today

IISER Pune is spread over a 100-acre area in Pashan, an educational and research hub of Pune, with several premier academic organizations in the vicinity.

Pune is connected by Air to all major cities across the country. The airport at Lohegaon doubles as an air force base. Pune is also well connected by trains and is accessible from Mumbai by road, which is a 3-hour drive. The Mumbai international airport has a regular taxi service to Pune. Regular bus service runs between the two cities as well.

Pune hosts a series of annual music festivals ranging from Indian Classical to Jazz and is home to renowned artists, musicians, and theatre groups that stage plays in Marathi and English. With the west coast just a couple of hours of drive away from Pune, several richly bio-diverse ecological hot spots are within reachable distances to Pune as are some of the spectacular beaches in this part of the country.

INDIAN INSTITUTE OF SCIENCE EDUCATION AND RESEARCH (IISER) PUNE
Dr. Homi Bhabha Road, Pashan, Pune-411008, India
Phone: +91-20-25908001; Fax: +91-20-20251566
Website: www.iiserpune.ac.in