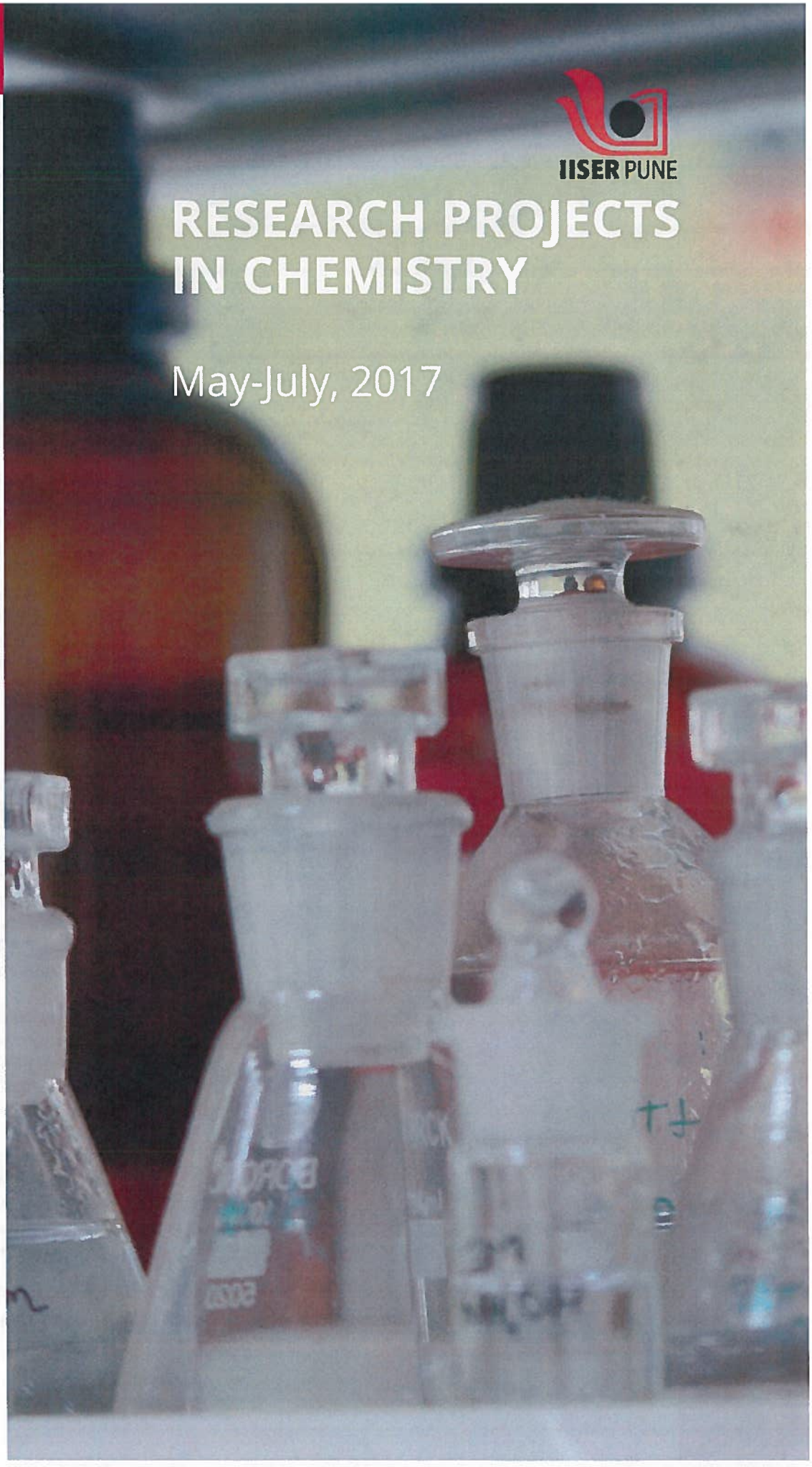
IISER PUNE - TEMPLE UNIVERSITY
SUMMER PROGRAM 2017



IISER PUNE

RESEARCH PROJECTS IN CHEMISTRY

May-July, 2017

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 2017 as part of this Program.

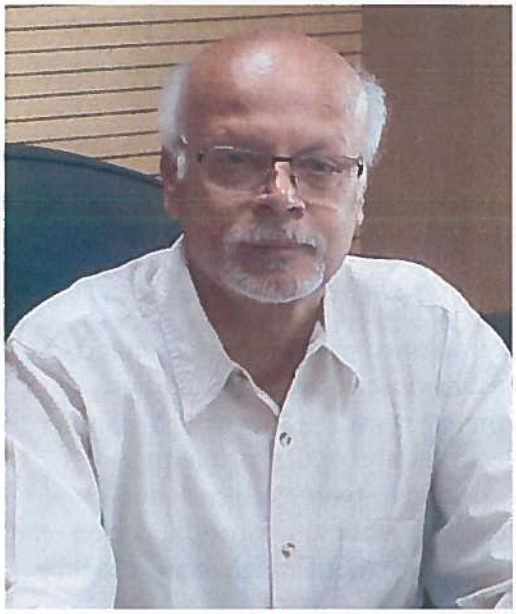
Applications: Interested students should directly contact the Project Investigator of interest. The initial inquiry should include a resume/CV, a transcript and a statement describing prior research experience, career goals and why the particular project is of interest.

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: Prof. K. N. Ganesh

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

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.

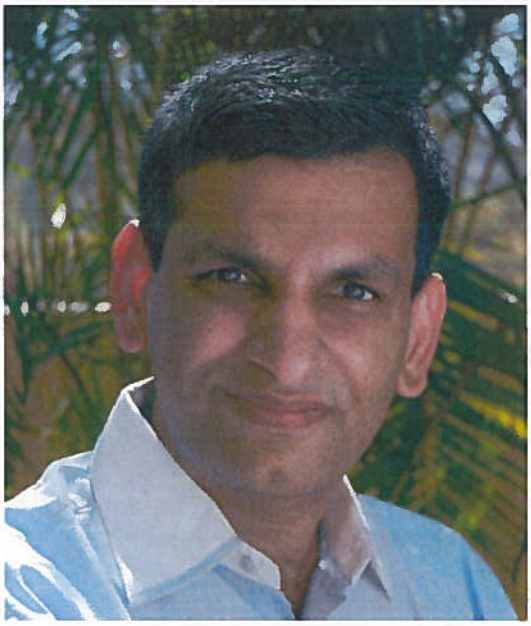
Research summary: Colloidal cesium lead halide perovskite Nanocrystals have been recently established as a new kind of defect-tolerant material, exhibiting interesting optoelectronic properties. Presently, we are doping various metal ions such Mn^{2+} and Bi^{3+} in such nanocrystals, for tailoring electronic 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/



COMPUTER SIMULATION OF NUCLEATION OF CLATHRATE HYDRATES: AN ENERGY STORAGE INITIATIVE

Project Investigator: Dr. Arun Venkatnathan

Preferred scientific requirements: Course in computational/quantum chemistry and/or hands on computer programming experience is preferred.

Research summary: Research in my group focuses on applying computer simulation methods to examine soft materials for energy conversion, storage and carbon capture. Our group examines a broad set of materials with emphasis on fuel cell membrane modelling and simulations, ionic liquids as charge carriers and carbon capture materials and understanding stability and formation of clathrate hydrates. The current project is focused on using simulations based on classical or reactive force-fields to explore possible mechanisms associated with nucleation and growth of clathrate hydrates.

Representative Publications

1. P. Prakash and A. Venkatnathan, Molecular mechanism of CO2 absorption in Phosphonium Amino Acid Ionic Liquid, RSC Advances, 6, 55438 - 55443 (2016). M. Kumar and A. Venkatnathan, Quantum Chemistry Study of Proton Transport in Imidazole Chains, J. Phys. Chem. B, 119, 3213 (2015). (Ionic Liquids)
2. 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). 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). (PEM Fuel Cells)
3. K. R. Ramya, G. V. Pavan Kumar and A. Venkatnathan, Raman spectra of vibrational and librational modes of methane clathrate hydrates using Density Functional Theory, J. Chem. Phys., 136, 174305 (2012). K. R. Ramya and A. Venkatnathan, Stability and Reactivity of Methane Clathrate Hydrates: Insights from Density Functional Theory, J. Phys. Chem. A, 116, 7742 (2012). (Clathrate Hydrates)

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

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

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

Project Investigator: Dr. Seergazhi G. Srivatsan

Preferred scientific requirements: Basic knowledge and preferable hands on experience in organic synthesis and molecular biology.

Research summary: Our group has been 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 ON sequences and study their structure and ligand-binding ability in cell models.

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. Nucl. Acid. Res. 2015, 43, e149.
2. Sawant, A. A.; Tanpure, A. A.; Mukherjee, P. P.; Athavale, S.; Kelkar, A.; Galande, S.; Srivatsan, S. G. A versatile toolbox for posttranscriptional chemical labeling and imaging of RNA. Nucl. Acid. Res. 2016, 44, e16.
3. 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.
4. Nuthanakanti, A.; Boerneke, M. A.; Hermann, T.; Srivatsan, S. G. Structure of the Ribosomal RNA Decoding Site Containing a Selenium-Modified Responsive Fluorescent Ribonucleoside Probe. Angew. Chem. Int. Ed. 2017, DOI: 10.1002/anie.201611700.

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


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.

IISER PUNE

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