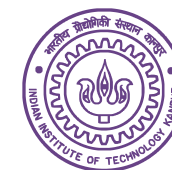


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## Department of Chemistry

Indian Institute of Technology Kanpur



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# IIT Kanpur

**I**ndian Institute of Technology Kanpur is engaged in carrying out original research of significance and technology development at the cutting edge. It imparts training to students so that they become competent and motivated engineers and scientists. The institute celebrates freedom of thought, cultivates vision and encourages growth, but also inculcates human values and concern for the environment and the society. The institute provides a wealth of resources in terms of both equipment and expertise. Our highly specialized laboratories, state-of-the-art design and testing facilities, advanced computing platform, and perhaps the best technical library in India can be shared to mutual benefit. The institute is open to establishing new partnerships with industry leaders and scholars of repute, cutting across all borders and barriers. The institute has now a total of 14 academic departments and five Inter-Disciplinary Programs (IDPs).

The Act of Parliament was passed in 1959 and IITK was established as a society in November, 1959. During the first ten years of its existence, IIT Kanpur benefited from the Kanpur Indo-American Program (KIAP), where a consortium of nine US universities namely M.I.T, University of California at Berkeley, California Institute of Technology, Princeton University, Carnegie Mellon University, University of Michigan, The Ohio State



University, Case Western Reserve University, and Purdue University helped to set up the research laboratories and academic programs. It is said to be the largest ever academic assistance program supported by the U.S.A. Such close interaction brought fresh air, new ideas and novel thoughts into the academic programs and academic administration.



# Message from the Chair

**T**he *Department of Chemistry* at the Indian Institute of Technology Kanpur is one of the premier teaching and research departments in the country. The department started its journey in early nineteen sixties under the leadership of Professor C.N.R. Rao and maintained vigorous momentum under a galaxy of exceptionally gifted faculty members over these years. Altogether, they propelled the department forward and put it firmly on the path of excellence in modern chemistry teaching and research.

Over the years, the department has been able to maintain a steady growth by not only increasing visibility in academics, but also by leading in the chemical sciences research landscape in India. This has been made possible by the collective efforts of dedicated faculty members, motivated students and committed supporting staff. Since its inception, the department has attracted world class faculty members, who are involved in all major areas of chemistry research. Several of our faculty members are also engaged in inter-disciplinary research spanning fields such as biology, physics and materials science. We offer a challenging environment for teaching and research in order to inculcate excellent working relationships with undergraduate and graduate students.

The department has several state-of-the-art

instruments to support cutting-edge research activities. Moreover, we have access to the excellent facilities in other departments and centers across the Institute. The Institute also provides other infrastructural support in various forms, such as central machine shop, glass-blowing section, central library and high-performance computing facility. Together, they support all research missions of the department.

For the last several decades, the department of chemistry has been a role model for academic programs throughout the country. This is due to the quality education imparted to the students at both undergraduate and postgraduate levels and excellent student-teacher relations. The accomplishments of our alumni reflect the high quality training imparted during their sojourn here, as many of them occupy prominent positions in academia and industry all over the world. Our faculty members have been recognized nationally and internationally for their excellent contributions to research and teaching.

As India progresses towards becoming a global power, aspirations of the society as well as demands of the industry are undergoing significant changes. Keeping these in perspective, the department is committed, with active support from the Institute as well as various funding agencies, to be at the forefront of exciting changes through high quality teaching and research

Prof. Sandeep Verma  
Head, Department of Chemistry  
IIT Kanpur





# Academic Programs

**T**he academic programs and teaching profile of the department are designed to cater to the diverse needs of the institute student community. Whether it is for a doctoral student seeking knowledge at the forefront of modern research, or a master student seeking to establish the fundamentals, or an undergraduate student of another department seeking to broaden his/her horizons, the Chemistry department offers suitable courses and programs to meet the needs. The department runs Undergraduate, Masters and Doctoral programs along the lines of the premier academic institutions of the world. In addition, it also offers masters, dual majors and minors to students of other departments.

## Undergraduate Programs

### Bachelor of Science

The department runs a 4-year Bachelor of Science (B.Sc.) program admitting students who have completed their high-school/intermediate college. Admission to the program is through the highly-competitive nation-wide examination, referred to as the Joint Entrance Examination (JEE). The B.Sc. program is very flexible and allows students to opt for courses according to their needs. There is a compulsory component of the program that includes basic courses in chemistry, mathematics, physics, life-sciences, humanities and social sciences. Other courses include electives in chemistry and open electives offered by other departments. Interested students can also take up research projects as part of their curriculum and also have the option of spending an additional year to earn a Masters degree. The students graduating from this program are well-equipped to further their career ambitions in higher studies, industries, management or public service sectors.

### Master of Science

The department runs a Master of Science program for students who have completed their bachelors degree in chemistry elsewhere. These students enter through a national-level examination called the Joint Admission Test to M.Sc. (JAM). The students take a combination of compulsory and elective courses and are required to carry out research work as part of their curriculum. Most of these students opt for higher studies in chemistry at many of the top institutions worldwide.

### Minors and Dual-majors

Undergraduate students in other departments of IIT Kanpur can take a set of chemistry courses and obtain minor degrees. Currently, the chemistry department

offers minors in Inorganic, Organic and Physical chemistry. Additionally, students from other departments can opt for a dual-major by taking a required set of courses during their undergraduate studies.



## Doctoral Program

The doctoral program of the chemistry department has over 250 students working with various research groups. The students are considered for this program once they clear either of the two nation-wide qualifying examinations post M.Sc. They are admitted in after a rigorous interview by a selection committee which is normally held twice a year. Typically, the students complete the doctoral program in about 5 years and are absorbed in industry, academia or post-doctoral research elsewhere.

# Teaching and Courses

**T**he *Chemistry department* is strongly committed to good teaching practices like a healthy teacher-student ratio, adequate teaching and laboratory assistantship, regular conduct of classes, continuous evaluation and a transparent system of grading.

## Types of Courses

### Core courses

A general chemistry classroom course and a general chemistry laboratory course are taught for all undergraduate students of IIT Kanpur.

### Chemistry option courses

These are optional courses offered to undergraduate students from different streams to give them an exposure to particular topics in chemistry.

### Departmental compulsory courses

The curricula for the B.Sc., M.Sc. and Ph.D. program have a component of compulsory course work, tailored to the requirements of the students in the program. In addition to classroom courses, some laboratory courses are also included.

### Department elective courses

These are optional courses that are taken by students in different programs depending on their field of interest.



Many of them are also taken by students from other departments whose interests match with that of the course.

### Project courses

Both the B.Sc. and the M.Sc. programs have research project courses in which, the students work with selected supervisors.



# Research Opportunities

**T**he *Department of Chemistry at IIT Kanpur* is renowned as a premier destination for chemistry research. The department is now a home to a number of researchers working in frontline areas in various aspects of chemical sciences. There are about 34 faculty members with research interests spanning the domains of inorganic, organic and physical chemistry. The research activities in the department encompass a vast expanse of traditional as well as interdisciplinary fields as detailed below.

## Inorganic Chemistry

The research interests of inorganic section span diverse areas that include coordination chemistry, bio-inorganic chemistry, organometallic chemistry, catalysis, and supramolecular chemistry. The study of inorganic entities in biological systems is also a major topic of interest, which includes studies on heme centers in heme protein and topics related to medicinal inorganic chemistry. The creation of new chemical entities with interesting structures, magnetic and electrochemical properties for applications in catalysis and material chemistry is also being pursued in many laboratories.

## Organic Chemistry

Research areas in organic chemistry include an eclectic mix of traditional and contemporary fields such as bioorganic chemistry, new reaction development, natural product synthesis, photochemistry, chemical biology, organic materials and catalysis. In addition to studying the chemistry of small molecules, the synthesis and application of carbohydrate and peptide based architectures and metal-organic frameworks for applications in medicine and material science are also being performed in a number of laboratories. Many laboratories are engaged in interdisciplinary research wherein chemical synthesis of new molecules is guided by their applications as modulators of biological function or as potential new catalysts and materials. Investigations of mechanistic basis of organic photo- and thermal reactions and development of organic functional materials based on de novo approaches are actively pursued.

## Physical Chemistry

Research areas in the domain of physical chemistry encompass computational and theoretical chemistry, reaction dynamics, spectroscopy, and materials chemistry. Specific areas include fundamental gas phase molecular dynamics, statistical mechanics, and the application of modern techniques like ultrafast pulse-shaping, molecular beams, single molecule spectroscopy and imaging, and fluorescence

correlation and up-conversion to study challenging problems involving electronic structure and dynamics. Both experimental and theoretical research components are strongly represented, and many research programs amalgamate a variety of techniques to answer fundamental questions.

## Inter disciplinary Research

Modern research problems are increasingly becoming multifaceted, and require research efforts that encompass more than one field of science. Our department has a number of laboratories involved in investigating such problems that lie on the interface of two disciplines, and incorporate research from synthetic chemistry, biological sciences, material sciences, medicinal chemistry, and drug discovery





# Faculty Profiles

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# Ganapathi Anantharaman



## ASSISTANT PROFESSOR

Born in Chennai, Tamil Nadu, 1976. M. Sc., IIT Bombay, 1999; Ph. D., University of Goettingen, Germany, 2004.

Joined as Lecturer, IIT Kanpur, 2004; Assistant Professor, IIT Kanpur, 2007.

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Coordination Polymers Built with Transition Metal Sulphates and Angular 2,5-bis(imidazol-1-yl)thiophene(thim<sub>2</sub>): Synthesis, Structure and Photoluminescent Properties, Cryst. Eng. Commun., 16, 6203 (2014)

Structural Diversity and Luminescent Properties of Coordination Polymers Based on Mixed Ligands, 2,5-Bis(Imidazol-1-yl)Thiophene(Thim<sub>2</sub>) and Aromatic Multicarboxylates, Cryst. Eng. Commun., 16, 7914 (2014)

A Hexameric Hexagonal Organotin Macrocycle. Supramolecular Entrapment of Iodide Anions with a Short Contact, Cryst. Growth. Des. 14, 3182 (2014)

Backbone Thio-Functionalized Imidazol-2-ylidene-Metal Complexes: Synthesis, Structure, Electronic Properties, and Catalytic Activity, Organometallics 32, 7006 (2013).

Synthesis and Characterization of NHC-Stabilized Zinc Aryloxide and Zinc, Organometallics 26, 1089 (2007)

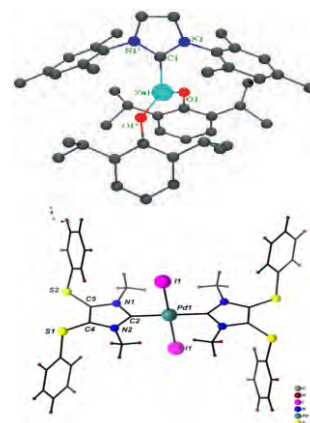
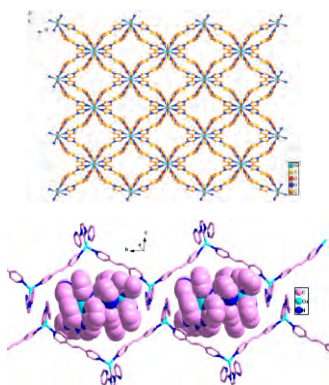
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Control of molecular topology and metal nuclearity in multimetallic assemblies: Designer metallocloxanes derived from silanetriols, Chem. Eur. J. 10, 4106 (2004)

Reactions of 2-Mercapto-benzoic Acid with Divalent Alkaline Earth Metal Ions: Synthesis, Spectral Studies, and Single-Crystal x-ray Structures of Calcium, Strontium, and Barium Complexes of 2,2'-Dithiobis(benzoic acid), Inorg. Chem. 40, 6870 (2001)

Catalysis plays an important role in life cycle. The natural catalysts present in our system, not only involves in the chemical transformation, but they are also recycled. The heterogeneous catalysts are good for organic transformation, but high quantity of catalysts is used and it has poor selectivity. In contrast the homogeneous catalysts are very good but suffer poor recyclability. Thus there is a great amount of thrust given to develop the heterogenization of homogeneous catalysts and as a result new supported catalysts with well defined positions of supporting units are being developed. Thus this work involves three broad area of Inorganic chemistry, namely (i) coordination polymers (ii) Organometallics, and (ii) homo- and/heterogeneous catalysis. Besides we want to study the materialistic aspects of the support and house the important materials inside the cavity. Therefore, in the first part, we are involved in developing the supports which is essential to (a) incorporate molecular

catalysts (b) carryout reactions inside the channels and (c) the study of material applications in the area of sorption and luminescence. In this regard, we have chosen heterocyclic ring containing linkers, such as pyridine and thiophene, imidazolium ions to prepare coordination polymers with different metal ions. Compared to the other heterocyclic ring systems or other two electron donors, NHCs are one of the versatile ligands used in the molecular catalysts for the organic transformation (organometallic chemistry and catalysis). In the catalysts preparation, understanding the electronic property of NHCs are necessary. Therefore, in recent years, we have been also engaged in the synthesis and reactivity of NHCs/modified NHCs, which are precursors for the linkers in the preparation of CPs, apart from understanding the electronic nature of NHCs. These expertises will be used later for the preparation of supported catalysts.



# Raja Angamuthu



## ASSISTANT PROFESSOR

Born in Karur, Tamilnadu, 1980. M. Sc., 2002; Ph. D., Leiden University, Leiden, The Netherlands, 2005-2009.

RA, Bharathidasan University, Tiruchirappalli, 2002-2005; University of Illinois at Urbana-Champaign, Rubicon Post Doctoral Fellow (from The Netherlands Organisation for Scientific Research, NWO), 2010-2012.

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Organo Ruthenium–Nickel Dithiolates with Redox-Responsive Nickel Sites, *Organometallics* 2013, 32, 6324.

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Electrocatalytic CO<sub>2</sub> Conversion to Oxalate by a Copper Complex, *Science* 2010, 327, 313.

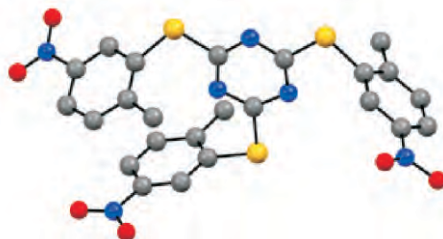
A molecular cage of nickel(II) and copper(I): a [(Ni(L)<sub>2</sub>)<sub>2</sub>(CuI)<sub>6</sub>] cluster resembling the active site of nickel-containing enzymes, *Chem. Comm.* 2009, 2700.

Reduction of protons assisted by a hexanuclear nickel thiolate metallacrown: protonation and electrocatalytic dihydrogen evolution. *Phys. Chem. Chem. Phys.* 2009, 11, 5578.

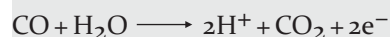
Hexanuclear [Ni<sub>6</sub>L<sub>12</sub>] metallacrown framework consisting of NiS<sub>4</sub> square-planar and NiS<sub>5</sub> square-pyramidal building blocks. *Dalton Trans.* 2007, 4641.

Laboratory of Inorganic Synthesis and Bio-Inspired Catalysis (LISBIC) walks along with nature to answer number of longstanding questions.

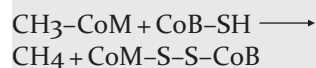
Our primary goals are to understand the structure and functions of organometallic active sites in enzymes such as Carbon Monoxide Dehydrogenase (CODH), Acetyl-Coenzyme A Synthase (ACS), Acireductone Dioxygenase (ARD), Methyl-Coenzyme M Reductase (MCR), Methyleneurease (MDU) and on top of all, Hydrogenase (H<sub>2</sub>ase), in order to develop simple small molecular models as catalysts for industrially and environmentally important chemical transformations such as (1) reversible interconversion of carbon dioxide and carbon monoxide, (2) decomposition of the acetyl group into separate one-carbon units or catalysing acetate synthesis using one-carbon unit precursors (3) C-C bond cleavage, (4) methane generation or activation, (5) degradation of methyleneurea (slow release fertilizer), and most prominently, (6) reversible interconversion of dihydrogen into protons and electrons. SO<sub>2</sub> sequestration and activation is one of our branching projects where we are developing molecules with multiple nucleophilic centers to bind with SO<sub>2</sub>.



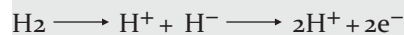
## Carbon Monoxide Dehydrogenase (CODH)



## Methyl-Coenzyme M Reductase (MCR)



## Hydrogenases (H<sub>2</sub>ase)





# Jitendra K. Bera



## PROFESSOR

Born in Tamluk, West Bengal, 1968. M. Sc., Kalyani University, 1993; Ph. D., Indian Institute of Science, Bangalore, 1999.

Purdue University, 1999-2001; Texas A&M University, 2001-2003; Assistant Professor, IIT Kanpur, 2003-2007; Associate Professor, IIT Kanpur, 2008-2011; Professor, IIT Kanpur, 2011 onwards; Fellow, Indian Academy of Sciences, 2013; Fellow, National Academy of Sciences, 2014.

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Amide-Functionalized Naphthyridines on RhII-RhII Platform: Effect of Steric, Hemilability and H-Bonding on Structural Diversity and Catalytic Activity of Dirhodium(II) Complexes, *Chem. Eur. J.* 20, 16537 (2014).

A Highly Efficient Catalyst for Selective Oxidative Scission of Olefins to Aldehydes: Abnormal-NHC-Ru(II) Complex in Oxidation Chemistry, *J. Am. Chem. Soc.*, 136, 13987 (2014).

Metal-Ligand Cooperation on a Diruthenium Platform: Selective Imine Formation via Acceptorless Dehydrogenative Coupling of Alcohols with Amines, *Chem. Eur. J.* 20, 6542 (2014)

Bulky, Spherical and Fluorinated Anion BArF Induces 'On-Water' Activity of Silver Salt for the Hydration of Terminal Alkynes, *Tetrahedron Lett.* 2014, 55, 1444.

Room Temperature C-H Bond Activation on a [PdIPdI] Platform, *Chem. Commun.* 2013, 49, 9764.

Cyclometalations on Imidazo[1,2-a][1,8]naphthyridine Framework, *Organometallics* 2013, 32, 4306.

Reactions of Acids with Naphthyridine-Functionalized Ferrocenes: Protonation and Metal Extrusion, *Inorg. Chem.* 2013, 52, 1432. Understanding C-H Bond Activation on a Diruthenium(I) Platform, *Organometallics* 2013, 32, 340.

A Non-Innocent Cyclooctadiene (COD) in the Reaction of 'Ir(COD)(OAc)' Precursor with Imidazolium Salts, *Organometallics* 2013, 32, 192.

Carbon Monoxide Induced Double Cyclometalation at the Iridium Centre, *Organometallics* 2012, 31, 5533.

Bera group at IIT Kanpur studies organometallic catalysts for small molecule activation and organic transformations. Towards this effort, organometallic compounds based on bimetallic constructs (M-M) are developed and their catalytic utility in organic reactions is explored. Dicopper (I), diruthenium (I) and dipalladium(I) compounds are synthesized which show excellent catalytic activity for cycloaddition, carbene transfer and C-C coupling reactions, respectively. Carefully designed experiments reveal that metal-metal cooperation influences substrate activation, guides stereoelectronic factors and promotes product elimination in the catalytic cycle. Lessons learnt from these studies are utilized to develop new-generation catalysts for conversion of cheap and abundant molecules to useful chemicals.

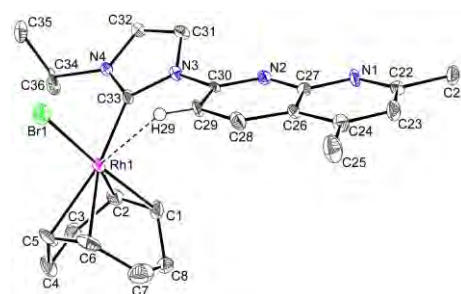
Another key area of research that is being developed at Kanpur includes designed catalysts featuring metal-ligand (M...L) cooperation. Carefully designed ligand scaffold which holds the metal ion and simultaneously offers proton-acceptor has been devised for bifunctional water activation. Using this principle, hydration, hydrolytic and oxidation catalysts that utilize water as a reagent is developed. The metal-ligand cooperation strategy is a simple and effective paradigm in small-molecule-activation chemistry. Importantly, it involves bifunctional substrate activation, and not necessarily oxidative addition/reductive elimination sequence, thus offering prospect for catalysts based on 3d metals. We are

presently developing catalysts that employ hydroxy / hydroxide and amine / amide functionality for activation of alcohol and hydrogen respectively.

Further, we seek to understand fundamental processes involved in organometallic reactions. Activation of C-H bond has remained a favorite topic in our research.

A host of experimental techniques including X-ray, NMR, GC-MS, kinetic studies, isotope labeling experiments are routinely carried out for compound characterization, and for studying reaction mechanism. Computational tools are often exploited to support proposed pathway. Through such unifying approaches, Bera group seeks to gain clear mechanistic understanding of chemical processes.

Recently, we have initiated a green chemistry program to address energy, environmental and sustainability aspects of chemical synthesis.



# Parimal K. Bharadwaj



## PROFESSOR

Born in Purulia, West Bengal, 1951. M. Sc., IIT Kharagpur, 1974; Ph. D., IIT Kharagpur, 1979.

UNESCO Fellow, Tokyo Institute of Technology, 1979-1980; postdocs: Rutgers University, 1980-1985; University of California at Davis, 1985-1987; Assistant Prof., 1987-1993; Associate Prof., 1993-1995; Professor, IIT Kanpur, 1995-present; Visiting Prof., University of Saarland, Germany, 1998; POSTECH, S. Korea, 2000-2001; Fellow, Indian Academy of Sciences, 1998; Fellow, Indian National Science Academy, 2008; Poonam and Prabhu Goel Chair, 2011-; J. C. Bose National Fellow, 2011; Distinguished Alumnus, IIT Kharagpur, 2013; Fellow of the Royal Society of Chemistry, 2014.

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## Selected References

A Chemosensor Built with Rhodamine Derivatives Appended to an Aromatic via 1,2,3-Triazoles: Dual Detection of Aluminium and Fluoride/ Acetate anions, *Inorg. Chem.*, 52, 1161 (2013).

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Effect of Bulkiness on Reversible Substitution Reactions at Mn(II) Center with Concomitant Movement of the Lattice DMF: Observation Through Single-Crystal to Single-Crystal Fashion, *Chem. Eur. J.*, 16, 5070 (2010).

A Porous Coordination Polymer Exhibiting Reversible Single-Crystal to Single-Crystal Substitution Reactions at Mn(II) Center by Nitrile Guest Molecules, *J. Am. Chem. Soc.*, 131, 10942 (2009).

A Cryptand Based Chemodosimetric Probe for Naked Eye Detection of Mercury(II) Ion in Aqueous Medium and Its Application in Live Cell Imaging, *Chem. Commun.*, 4417 (2009)

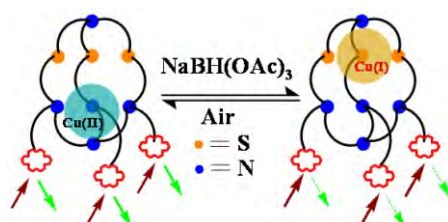
Translocation of Copper Within the Cavity of Cryptands: Reversible Fluorescence Signaling, *Chem. Commun.*, 4180 (2008)

The principal thrust of present research activities has been in the area of supramolecular chemistry of cryptands and coordination polymers for various applications

### (i) Cryptand:

Made a new synthetic protocol for multigram synthesis of cryptands adopted by others.

Major contributions include transition metal induced fluorescence enhancement. Transition metal ions that are known as effective quenchers, can give large enhancement with cryptand based systems. Such systems are useful as sensors for biological/ environmental applications and as logic gates for molecular information processing. Another important research is based on cryptand based new generation of amphiphiles for stable Langmuir-Blodgett films and vesicular aggregates. Translocation of a metal ion inside the cavity as well as inside to outside of the cavity in a reversible manner has been achieved.

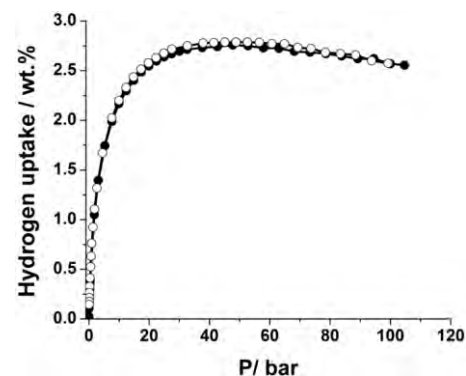
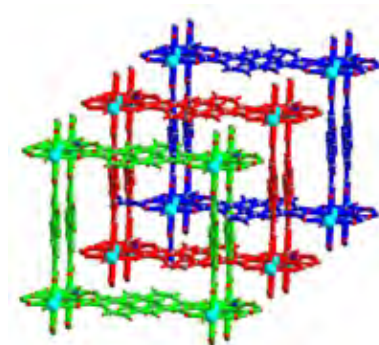


Presently, we are engaged in single- as well as multi- step FRET and use of cryptands as platforms for attachment of donors and acceptors for charge separation. Besides, new generation of cryptands for exocyclic coordination are also being pursued.

### (ii) Coordination Polymers:

Research activity in this emerging area of chemistry involves synthesis of coordination polymers and use them to store gases for mobile applications. In addition various other applications such as heterogeneous catalysis, separation of geometrical isomers, magnetism, proton conductance and so on are being investigated.

In a major thrust, single-crystal to single-crystal (SC-SC) transformations of coordination polymers for various applications are being probed.





# Amalendu Chandra



## PROFESSOR

Born in Burdwan, West Bengal, India, 1963. M. Sc., University of Burdwan, 1986; Ph.D. Indian Institute of Science, Bangalore, 1991.

Postdoctoral Fellow, University of British Columbia, 1991-93; Assistant Professor, 1993-1999; Associate Professor, 1999-2001; Professor, IIT Kanpur, 2001-present; Sajani Kumar Roy Memorial Chair Professor, IIT Kanpur, 2011-2014; Shanti Swarup Bhatnagar Prize, CSIR, 2007; Fellow, Indian Academy of Sciences, 2006; Fellow, Indian National Science Academy, 2013; J. C. Bose National Fellow, 2013.

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## Selected References

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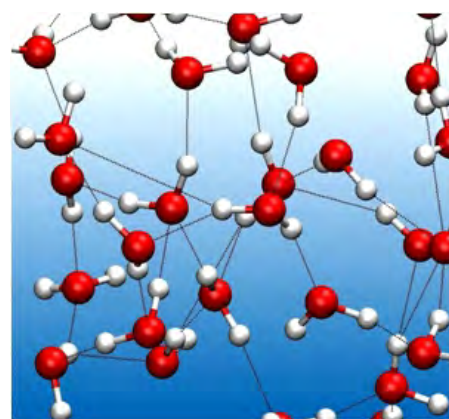
J. Chem. Phys. 115, 3732 (2001).

Effects of ion atmosphere on hydrogen-bond dynamics in aqueous electrolyte solutions, Phys. Rev. Lett. 85, 768, (2000).

Our research interests include studies of equilibrium and dynamical behaviour of complex molecular liquids and ionic solutions in bulk, at interfaces and in confined environments and also of molecular clusters based on theoretical and computational methods. We have been working on (i) Structure and dynamics of hydrogen bonds and their relations to vibrational spectral diffusion in associated liquids, (ii) Molecular and collective dynamics and dielectric decrement of electrolyte solutions at high ion concentrations, (iii) Structure, dynamics and polarity of molecular liquids at solid-liquid and liquid-vapour interfaces and in confined environment, (iv) Behaviour of molecular solutions under extreme conditions, (v) Hydration and translocation of protonic defects in aqueous systems and (vi) Electron localization in molecular liquids and clusters. Our work includes both development of theories based on modern statistical mechanical methods as well as applications of state-of-the-art simulation techniques.

Studies of hydrogen bond dynamics in associated liquids constitute a major area of our research in recent years. We showed how the presence of ions affects the structure and dynamics of hydrogen bonds in aqueous systems. Very recently, we have gone beyond the use of pair potentials and has used the technique of Car-Parrinello molecular dynamics to study the relaxation of hydrogen bonds and associated vibrational spectral diffusion in aqueous and other associated liquids

from first principles without using any pair potentials. We have established the connections of observed spectral diffusion to underlying molecular dynamics of water molecules from first principles calculations.





# Manabendra Chandra



## ASSISTANT PROFESSOR

Born in Burdwan, West Bengal, India, 1979. Masters: The University of Burdwan, 2003; Ph. D., Indian Institute of Science, 2009.

Postdoctoral Fellow, Florida State University and National High Magnetic Field Laboratory, 2009-2013; Assistant Professor, IIT Kanpur, 2013-.

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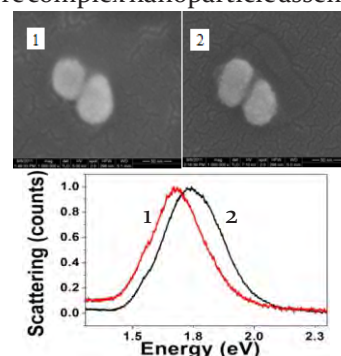
Controlled Plasmon Resonance Properties of Hollow Gold Nanosphere Aggregates, *J. Am. Chem. Soc.*, 132, 15782 (2010).

Small-particle limit in the Second Harmonic Generation from Noble Metal Nanoparticles, *Chem. Phys.*, 358, 203 (2009)

We are applying spectroscopic techniques to solve problems in nanoscience. One of our main focus areas is the study of localized plasmons of metallic and metal-based nanoparticles and nanostructures. The optical properties of these structures are quite fascinating, and include a strong effect of geometry on the optical resonant properties, size dependent effects controlling light absorption and scattering, and plasmon-plasmon interactions, as observed in reduced symmetry nanoparticles and finite nanoparticle aggregates. These latter systems are of particular interest, giving rise to a rich variety of coupled-oscillator behavior such as Fano resonances, electromagnetically induced transparency (EIT), sub- and superradiance, and many other interesting phenomena. Although these phenomena are of fundamental interest yet they have the potential to impact applied areas e.g., solar-energy conversion, advanced imaging techniques, forensics science, etc.

The excitation of a nanoparticle surface plasmon gives rise to absorption and scattering, and also creates a strong local electromagnetic field around the metal nanoparticle surface. Ensemble extinction spectroscopy measures the sum of both absorption and scattering and averages over all nanoparticle sizes and shapes present within the detection volume. To eliminate inhomogeneous broadening of the surface plasmon resonance due to distributions in particle size, shape, and environment,

as our main tool, we are using single-particle spectroscopy and imaging techniques to understand the radiative and nonradiative properties of individual plasmonic nanoparticles and their finite assemblies. Single particle spectroscopy, especially when correlated with structural imaging using electron microscopy, provides the ultimate resolution and has enabled major breakthroughs in materials chemistry and physics because heterogeneous distributions of nanoparticle shape, size, and orientation or interfacial nanoscale structure can be measured directly. The goal is to determine the plasmonic properties of anisotropic nanostructures that are used as sensors or biological probes and for comparison to more complex nanoparticle assemblies.



An example of structure-specific optical property of finite assembly of plasmonic nanoparticles: The figure above shows SEM images of two Au nanoparticle dimers and their dark-field scattering spectra. The same nanostructures are identified in the electron and optical microscopes using patterned substrates with identification marks.



## PROFESSOR

Born in Kolkata, 1958. M. Sc., Osmania University, 1977; Ph. D., Indian Institute of Science, 1982.

University of Massachusetts, Amherst, U. S. A., 1983-86; Indian Petrochemicals Corporation Limited, Vadodara, 1986-87; IIT Kanpur, 1987-present; Alexander von Humboldt Fellow, University of Göttingen, Germany, 1994-95; Wilhelm-Bessel Fellow, University of Göttingen, Germany, 2004; Tata Institute of Fundamental Research, Centre for Interdisciplinary Sciences, Hyderabad, 2012-14; Director, National Institute of Science Education and Research, Bhubaneswar, 2014.

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Pentanuclear Heterometallic  $\{Ni_2Ln_3\}$  ( $Ln = Gd, Dy, Tb, Ho$ ) Assemblies. Single-Molecule Magnet Behavior and Multistep Relaxation in the Dysprosium Derivative, *Inorg. Chem.*, 52, 13078 (2013).

Stabilizing the  $[Rn(\mu_2-O)SnR]$  Motif through Intramolecular  $N \rightarrow Sn$  Coordination. Synthesis and Characterization of  $[(Rn)(\mu_2-O)(\mu_2-O)FcCOO)_2](\eta-FcCOO)_2 \cdot THF$  and  $\{(Rn)_2(\mu_2-O)[(t-BuO)_2PO_2]_2Cl_2\} \cdot THF \cdot 2H_2O$  ( $R = 2-(Phenylazo)phenyl$ ), *Organometallics*, 32, 3419, (2013).

Molecular indium(III) phosphonates possessing ring and cage structures. synthesis and structural characterization of  $[In_2(t-BuPO_3H)_4(phen)_2Cl_2]$  and  $[In_3(C_5H_9PO_3)_2(C_5H_9PO_3H)_4(phen)_3] \cdot NO_3 \cdot 3.5H_2O$ , *Inorg. Chem.*, 52, 13078 (2013).

Molecular transition-metal phosphonates, *Dalton Trans.* 5394 (2011)

Phosphorus-Supported Ligands for the Assembly of Multimetal Architectures, *Acc. Chem. Res.* 42, 1047 (2009)

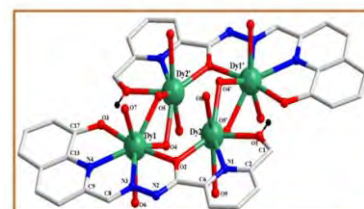
We work in the area of main-group organometallic chemistry, polynuclear metal complexes, inorganic rings, cages and polymers and in molecular materials. The common thread that connects all of these themes is synthesis and structure.

Inorganic rings and polymers provide an interesting platform for a synthetic inorganic chemist. Some of the inorganic rings can be converted to the corresponding high polymers. Alternately, inorganic rings can be stitched as pendants on organic polymer platforms. Both of these approaches are of interest to us and we widely investigate them particularly with respect to systems containing P-N motifs. Another aspect of interest is to use the inorganic rings and cages such as cyclophosphazenes or stannoxanes as scaffolds for building functional molecules. We have considerable interest in this field as it provides access to many novel assemblies possessing interesting electro- or photochemical properties. Also, such approaches are useful for preparing new hybrid nanomaterials that are catalytically active.

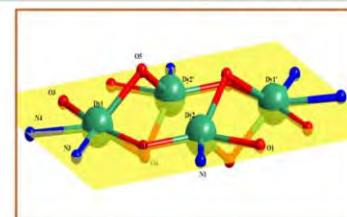
We are also interested in using inorganic motifs to support new multi-site coordinating ligands using which polynuclear complexes can be built. The interest in such systems emanates from their structure as well as properties. For example, the phosphonate family of ligands represented by  $[RPO_3]^{2-}$  afford, layered metal phosphonates. However, we have pioneered an ancillary ligand approach that allows molecular assemblies whose nuclearity can be modulated considerably.

Our interest in this is to be able to make new molecular materials such as single-molecule magnets (SMMs) as well as systems that are catalytically active. Our interest in main-group organometallic chemistry is to understand the M-C bond reactivity in these systems and using their lability to construct complex architectures.

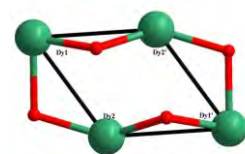
Our research programs are driven by fundamental questions whose solutions can also lead to emerging applications.



Molecular structure of  $[Dy_4(H_2O)_8(O)_4(LH_2)]$



Planar arrangement of the four  $Dy(III)$  ions



Rhombus shaped  $Dy_4$  core of 1; Bond distances:  $Dy1-Dy2'$ , 3.799 Å;  $Dy1-Dy2$  3.791 distance Å



# Dattatraya H. Dethe



## ASSOCIATE PROFESSOR

Born in Pune, Maharashtra, 1976. M. Sc., University of Pune, 1999; Ph. D., Indian Institute of Science, Bangalore, 2005.

ICES, A-STAR, Singapore, Research Fellow, 2005-2008; Albany Molecular Research Inc., Singapore, Senior Research Scientist, 2008-2009; Scientist E<sub>1</sub>, National Chemical Laboratory, Pune, 2009-2011; Assistant Professor, IIT Kanpur, 2011-2014, Associate Professor, 2014-.

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Remarkable switch of regioselectivity in Diels-Alder reaction: Divergent total synthesis of borreverine, caulindoles and flinderroles, *Org. Lett.*, 16, 2764 (2014).

Biomimetic total syntheses of borreverine and flinderole alkaloids, *J. Org. Chem.*, 78, 10106 (2013).

FeCl<sub>3</sub> mediated intramolecular olefin-cation cyclization of cinnamates for the synthesis of highly substituted indenenes, *Chem. Comm.*, 49, 8051 (2013).

Cu(OTf)<sub>2</sub> catalysed [6+2] cycloaddition reaction for the synthesis of highly substituted pyrrolo[1,2-a]indoles: rapid construction of yuremamine core, *Chem. Comm.*, 49, 3260 (2013).

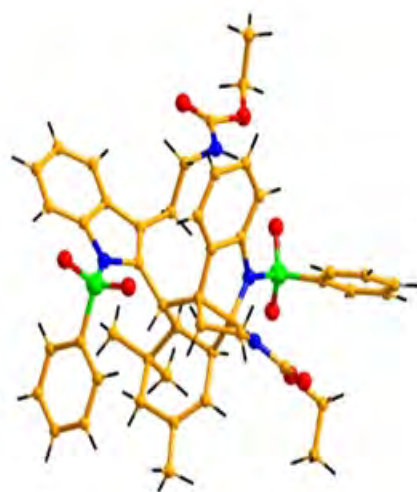
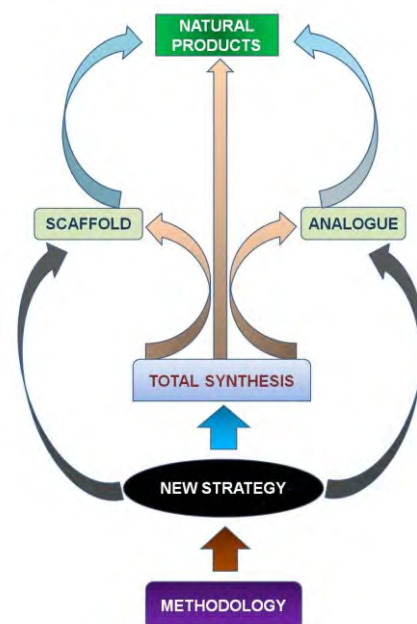
FeCl<sub>3</sub> Catalyzed Prins-Type Cyclization for the Synthesis of Highly Substituted Indenes: Application to the Total Synthesis of (±)-Jungianol and epi-Jungianol, *Org. Lett.*, 15, 429 (2013).

Asymmetric first total syntheses and assignment of absolute configuration of oxazinin-5, oxazinin-6 and preoxazinin-7, *Org. Biomol. Chem.*, 9, 7990 (2011).

Biomimetic total syntheses of flinderroles B and C, *J. Am. Chem. Soc.*, 133, 2864 (2011).

The total synthesis of natural products (usually biologically active) or organic compounds having theoretical interests in chemistry or biology is still as healthy and vigorous as ever. The journey of total synthesis was started in early nineteenth century. In the year 1828 Friedrich Wohler did the first total synthesis of urea, which can be considered as the birth of total synthesis. Now, in 21st century for the determination of structure and architecture of a molecule so many powerful techniques are established. These tools allow the chemists to think for the synthesis of some highly complex molecules which cannot be even imagined in the earlier era of organic synthesis.

The research of our group is mainly focused on the development of new synthetic methods and strategies, and their application in the total synthesis of natural products and biologically important compounds. A major thrust of our current research is the design and invention of new annulation strategies for the synthesis of carbocyclic and heterocyclic systems. Our research program is focused on the development of new reagents and methods for organic synthesis, with an emphasis on asymmetric catalysis. The achievement of our objectives requires an understanding of stereoselective synthesis, physical organic chemistry, and metal-based reactivity.





# Shridhar R. Gadre



## PROFESSOR

Born in Akola, India, 1950. M. Sc., The University of Pune, 1972; Ph. D., Indian Institute of Technology Kanpur, 1978.

Postdoctoral Research, UNC, Chapel Hill and University of Houston, 1978-1980; Lecturer and Professor, University of Pune, 1980-2010; Professor, IIT Kanpur, 2010-. Fellow, Indian Academy of Sciences, Bangalore, 1992; Fellow, Indian National Science Academy, New Delhi, 1996; Shanti Swarup Bhatnagar Award in Chemical Sciences, 1993; J. C. Bose National Fellow, 2007-.

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Facilitating Minima Search for Large Water Clusters at MP2 Level via Molecular Tailoring, J. Phys. Chem. Lett. 3, 2253 (2012).

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Some novel characteristics of atomic information entropies, Phys. Rev. A32, 2602 (1985).

The group of Professor Gadre is actively engaged in research in Quantum Chemistry. The research areas are as follows (with those of active current interest are highlighted):

- ☒ Electron density in momentum space
- ☒ Information Entropy in Quantum Chemistry
- ☒ Rigorous inequalities in Quantum Chemistry
- ☒ **Molecular Electrostatic Potential (MESP) and its Applications to Chemistry**
- ☒ **Development of Parallel ab initio Codes**
- ☒ **Molecular Clusters**

The use of the scalar field of molecular electrostatic potential (MESP) offers understanding of molecular reactivity and binding patterns for weak intermolecular interactions. Some basic theorems on topographical characteristics of MESP were proven in the group. This was followed by application of MESP and its critical points (CP) to a variety of chemical phenomena such as  $\pi$  facial selectivity, Hammett constants, Markovnikov's reaction, Clar's theory of aromatic sextets etc. Recently, MESP CPs have been employed for defining molecular recognition and lone pairs. Further, the lock-and-key features of MESP have been used for building up of large molecular clusters.

Development of parallel computing programs in quantum chemistry has been a long term interest of the group. The group has had long association with the **Centre for Development of Advanced Computing (C-DAC) Pune**,

The latest software development includes **Molecular tailoring approach (MTA)** for ab initio treatment of large molecules at high level of theory, which is difficult to carry out by employing standard packages. The current version of MTA enables electronic energy estimation, geometry optimization, evaluation of energy gradients and Hessian etc. A recent development includes a Molecular Cluster Builder for generating structures of large clusters from smaller ones by adding a monomer. A related parallel package for many body interaction energy analysis of molecular clusters (MBAC) allows systematic analysis of clusters. Earlier efforts include development of parallel quantum chemistry codes INDMOL, INDPROP and electrostatics based model (EPIC) to study weak intermolecular interactions. Members of the group with computer science background have developed excellent visualization softwares (UNIVIS) and MeTA Studio. MeTA Studio also facilitates fragmentation of molecules needed for running MTA jobs.

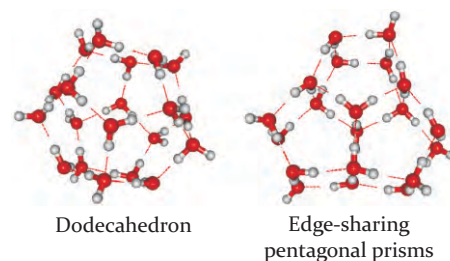


Figure: MTA optimized geometries of  $(\text{H}_2\text{O})_{20}$ .

# Namdeo S. Gajbhiye



## PROFESSOR

Born in Nagpur, Maharashtra, 1952. M. Sc., Nagpur University, 1975; Ph. D., IISc Bangalore, 1981.

Assistant Professor, IIT Kanpur, 1982-1992; Associate Professor, IIT Kanpur, 1992-1999; Professor, IIT Kanpur 1999-, DAAD Fellow (German Academy of Science), 1996; Fellow, World Innovation foundation, U. K., 2001. Fellow, National Academy of Science, Allahabad, 2002.

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Structural transformation and enhancement in magnetic properties of single-phase  $\text{Bi}_{1-x}\text{Pr}_x\text{FeO}_3$  nanoparticles, *J. Appl. Phys.* 113, 203917 (2013).

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Synthesis and Characterization of Self-assembled Nanofiber-bundles of  $\text{V}_2\text{O}_5$ : Their Electrochemical and Field Emission Properties, *Nanoscale* 4, 645 (2012).

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Electronic and magnetic properties of ligand-free FePt nanoparticles, *Adv. Mater.* 17, 574 (2005).

Magnetic Properties of  $\epsilon\text{-Fe}_3\text{N}$ -GaN Core-Shell Nanowires, *Nanotechnology*, 16, 2012 (2005).

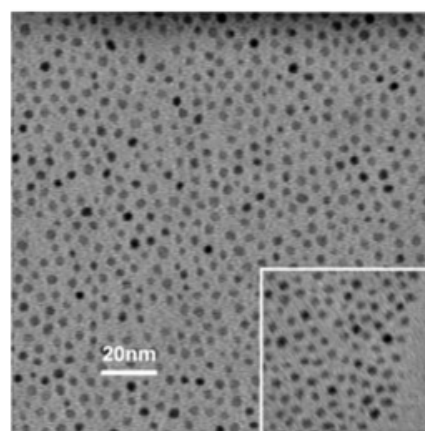
Research in the Gajbhiye group combines the use of synthetic, spectroscopic, magnetic, dielectric, and electrochemical experiments to advance the development of new multifunctional inorganic nanomaterials for spintronics, storage & memory devices, catalysis, contrast agents for MRI and Fluorescence imaging and energy conversion technologies. This research has components of inorganic, physical and materials chemistry cutting across all the interdisciplinary areas.

Nanoscience is the science of manipulating and controlling things on a small length scale of the materials; a scale of the order of size of the atoms and molecules. The technology behind the applications of materials in our lives is the nanotechnology. At present, nanotechnology is recognized in all fields of science and engineering.

Our research emphasizes application of a diverse array of complementary physical techniques to probe the electronic structures and physical properties of the new materials that we develop. Core experiments include X-ray diffraction, Fourier transform infrared, photoluminescence, Raman, X-ray photoelectron, Mössbauer spectroscopy, Electron paramagnetic resonance, and SQUID magnetometry, all over broad temperature ranges. Cyclic voltammetry and potentiometry are also used for the electrochemical lithium ion intercalation / de-intercalation characterization. Our group has a broad interest in areas: Self-assembly of monodispersed metal nanoparticles: Co, Fe, Ni, Ag, Co-Pt,

FePt, and composites.

Electronic and magnetic properties of nanostructured transition metal nitrides, oxides [Garnets, Spinel and Hexagonal Ferrites]. In depth study of defect chemistry in variety of morphologies of nanostructured CuO and  $\text{TiO}_2$  controls structure-property relations used for diluted magnetic semiconductor applications.



Original pure nanoparticles densely packed 2D arrangements of FePt nanoparticles.

N. S. Gajbhiye et. al. *Adv. Mater.*, 17, 574 (2005).



## PROFESSOR

Born in Midnapore, West Bengal, India, 1967. M. Sc., Indian Institute of Technology Kharagpur, 1991; Ph. D., National Chemical Laboratory, Pune (University of Pune), 1998.

Post-doctoral research associate, Wuerzburg University, Germany, 1998-1999; Alexander von Humboldt fellow, University GH Siegen, Germany, 1999-2000; Post-doctoral research associate, Massachusetts Institute of Technology, USA, 2001-2002; Assistant Professor, IIT Kanpur, 2002-2007; Associate Professor, IIT Kanpur, 2008-2011; Professor, IIT Kanpur 2011-.

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## Selected References

A Route to Highly Functionalized  $\beta$ -Enaminoesters via a Domino-Ring Opening-Cyclization-Decarboxylative Tautomerization Sequence of Donor-Acceptor Cyclopropanes with Substituted Malononitriles, *Org. Lett.*, 16, 2204 (2014).

Synthesis of 3,5-Disubstituted Cyclohex-2-en-1-one via a Five-Step Domino Reaction Catalyzed by Secondary Amines: Formation of (E)- $\alpha,\beta$ -Unsaturated Methyl Ketones, *Asian J. Org. Chem.*, 2, 1026 (2013).

An efficient synthetic route to carbocyclic enaminoitriles via Lewis acid catalysed domino-ring-opening cyclisation (DROC) of donor-acceptor cyclopropanes with malononitrile, *Chem. Commun.*, 49, 8205 (2013).

Memory of Chirality (MOC) Concept in Imino-Aldol Reaction: Enantioselective Synthesis of  $\alpha,\beta$ -Diamino Esters and Aziridines, *J. Org. Chem.*, 78, 2311 (2013).

A Synthetic Route to Chiral Indolines via Ring Opening/C-N Cyclization of Activated 2-Haloaryl-aziridines, *J. Org. Chem.*, 78, 3867 (2013).

Domino Imino-Aldol-Aza-Michael Reaction: One-Pot Diastereo- and Enantioselective Synthesis of Piperidines, *J. Org. Chem.*, 75, 7061 (2010).

Lewis Acid-Mediated Unprecedented Ring-Opening Rearrangement of 2-Aryl-N-tosylazetidines to Enantiopure (E)-Allylamines, *Org. Lett.*, 9, 5441 (2007).

Prof. Ghorai's research interests lie in the area of i) synthetic and mechanistic investigation of small ring aza-heterocycles, ii) enolate and dianion chemistry, and iii) asymmetric synthesis including natural products and drugs employing the concept of either memory of chirality, chiral pool or organocatalysis.

My group has demonstrated the MOC concept in imino-aldol reactions for the first time. We have been exploring MOC concept in a number of important chemical transformations e.g. aldol reaction, Michael reaction and many other domino processes.

We have established that the Lewis acid catalyzed nucleophilic ring-opening of 2-aryl-N-tosyl-aziridines or azetidines does proceed through an  $SN_2$ -type pathway instead of a stable 1,3- or 1,4-dipolar intermediate, respectively, as invoked earlier in the literature. We further demonstrated that non-nucleophilic quaternary ammonium salts could be employed in controlling the racemization process and it could be possible to obtain the ring opening products from aziridines and azetidines with an external nucleophile in the presence of a non-nucleophilic Lewis acid with enhanced diastereo- and enantioselectivity.

This finding enabled us to design and develop new innovative and creative synthetic routes towards various non-racemic bio- and pharmacologically active acyclic and cyclic compounds of contemporary interest. Very recently, we have successfully applied the methodology for donor-acceptor (DA)

cyclopropanes for the stereoselective synthesis of a number of carbacycles.

We have developed many new domino reactions e.g. domino-imino-aldol-aza-Michael, domino-aldol-Michael, domino-Michael-Michael via enolate anion and dianion chemistry. We have introduced a new concept, domino ring opening cyclization (DROC) for the stereoselective formation of carbacycles and aza/oxa- heterocycles employing activated aziridines, azetidines and DA-cyclopropanes with suitable nucleophiles.

Our research group has efficaciously employed metal- and organocatalysts in the field of domino reactions as well. Overall our research activities have provided new directions to organic synthesis in general and asymmetric synthesis in particular.





# Debabrata Goswami



## PROFESSOR

Born in Ichapur, West Bengal, 1964. M. Sc., IIT Kanpur, 1988; Ph. D., Princeton University, 1994.

PDF at Harvard University, 1995; Worked at Brookhaven National Labs, 1996; Quantronix Corporation, 1997; Princeton University, Center for Ultrafast Laser Labs, 1998; Tata Institute of Fundamental Research Mumbai, Fellow-E, 1999-2003; Associate Professor, IIT Kanpur, 2003-2009; Professor, IIT Kanpur, 2010-; Welcome Trust International Senior Research Fellow, 2004-2010; Swarnajayanti Fellow, 2005-2010; OSA Senior Member, 2012-.

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Effect of Molecular Structural Isomers in Thermal Lens Spectroscopy, Chem. Phys. Lett., 2014.

Controlling the femtosecond laser-driven transformation of dicyclopentadiene into cyclopentadiene, Chem. Phys. Lett., 558, 1 (2013).

Towards controlling molecular motions in fluorescence microscopy and optical trapping: a spatiotemporal approach, Int. Rev. Phys. Chem., 30, 275 (2011).

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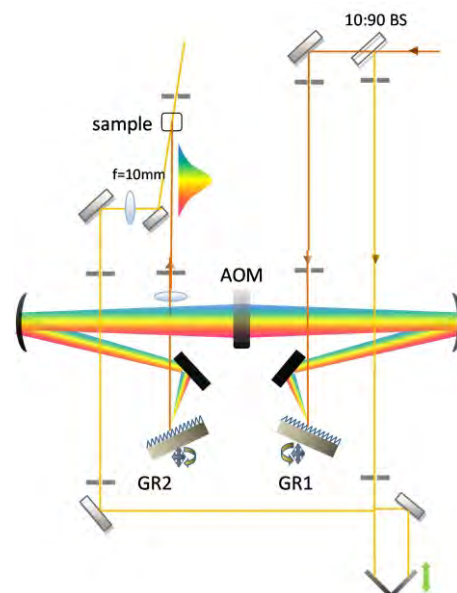
Laser phase modulation approaches towards ensemble quantum computing, Phys. Rev. Lett., 88, 177901 (2002).

Our research focusses on Femtochemistry and experimental coherent control for spectroscopic enhancement. This program addresses fundamental aspects of laser-matter interactions with arbitrary pulse shaping. We investigate ultrafast laser pulse shaping applications in gaseous and liquid phase molecular dynamics, optoelectronics, nonlinear optics and optical communication, biologically relevant multi-photon fluorescence microscopy and optical trapping. These diverse fields have been knit together for quantum information processing.

One of our approaches to exerting control over fundamental molecular processes has been in developing and exploring different control parameters that are systematically intrinsic: the environment around a molecule of interest plays a very important role. Molecules at the solid-liquid or liquid-liquid interface often behave in ways different from those observed in solution or in gas phase. Similarly, molecules under the influence of huge photon flux even at non-resonant interactive conditions behave distinctly. Likewise creating localized heating effects with femtosecond lasers gives rise to identifiable molecular signatures that have spectroscopic applications. We have also managed to show how to distinguish overlapping fluorophores in multiphoton imaging microscopy by exploiting repeated excitation and de-excitation processes with high repetitive rate femtosecond lasers. We have identified myriads of control parameters ranging from almost every laser parameter to the pH of the medium

being studied. From conditions arising in optically designed environments, we show that a system's behaviour stems from its organization at nano-scales. With such levels of understanding of control, we plan to process information at molecular levels to facilitate quantum information processing.

Thus the Goswami Group focusses on interdisciplinary areas of chemistry, biology and materials. A common region of interest in several of our programs is the interface between a material and a biological environment. We use programmable femtosecond laser pulses shaped to design and synthesize environments of our desired structures and properties. Hence the programs are adaptable to a large variety of problems addressing both fundamental and applied questions.



# Srihari Keshavamurthy



## PROFESSOR

Born in Bengaluru, India, 1967. M. S., Villanova University, 1989; Ph. D., University of California, Berkeley, 1994.

Cornell University, Postdoc, 1995 - 1996; Assistant Professor, IIT Kanpur, 1997-2003; Associate Professor, IIT Kanpur, 2003-2010; Professor, IIT Kanpur 2010-.

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## Selected References

Dynamical traps lead to the slowing down of intramolecular vibrational energy flow, *Proc. Natl. Acad. Sci., (USA)* **111**, 14354 (2014).

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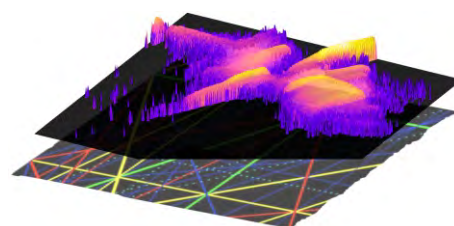
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Intramolecular vibrational energy redistribution as diffusion in state space: classical-quantum correspondence, *J. Chem. Phys.* **125**, 141101 (2006).

Resonance-assisted tunneling in three degrees of freedom without discrete symmetry, *Phys. Rev. E*, **72**, 045203 (2005).

Chemistry is all about making and breaking of bonds and the rate at which they do so. To break a specific bond all that has to be done is to excite that bond and dump energy in excess of the bond strength. With some luck the deposited energy will stay put for a few vibrational time periods (about a few hundred femtoseconds) and then the bond snaps. Turns out that this viewpoint is far too naive due to the fact that molecules excited to such high energies have complicated intramolecular dynamics. The excited mode is coupled to many other modes and thus the initially localized energy flows rapidly into many other, perhaps undesirable, modes. In other words, the molecular choreography is very complicated. Sometimes it is so complicated that it is simple! This flow of energy within a molecule is the phenomenon of Intramolecular Vibrational energy Redistribution (IVR). The questions that we are, as many other chemical physicists in the world are, interested in: Where does the energy flow? How? Why? How fast? How is this classical notion of ball-and-spring vibrational motion encoded in the quantum eigenstates? Explaining and hence understanding this molecular choreography will let us control molecular reaction dynamics. Our group is working on unraveling the IVR pathways in molecules from classical, semiclassical and quantum viewpoints. IVR is facilitated in a molecule by chains of nonlinear resonances which form a intricate

network - sort of a transport network complete with highways, by-lanes and dead-ends. What part of this network is utilized by the classical dynamics? An important question is whether the quantum dynamics respects the classical resonance network or does it use a shortcut, known as dynamical tunneling, to give rise to novel quantum IVR pathways. Perhaps, a detailed knowledge of this resonance road map will allow us to shut down some of the highways leading to controlled IVR and thus give mode-specific chemistry a fair chance to happen. Amongst other things, our research sheds new light on the mechanism of coherent control of gas phase reaction dynamics.



# Sabuj K. Kundu



## ASSISTANT PROFESSOR

Born in Hooghly, W.B., 1981. M. Sc., IIT Bombay, 2004; Ph. D., Rutgers, The State University of New Jersey, 2009.

University of Rochester, Postdoctoral Fellow, 2009-2011; The University of North Carolina at Chapel Hill, Postdoctoral Fellow, 2011-2013; DST INSPIRE Faculty, IIT Kanpur, 2013-.

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Cleavage of Ether, Ester and Tosylate C(sp<sup>3</sup>)-O Bonds by an Iridium Complex, Initiated by Oxidative Addition of C-H bond. Experimental and Computational Studies, *J. Am. Chem. Soc.*, 135, 5127 (2013).

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Synthesis of Piperylene and Toluene via Transfer Dehydrogenation of Pentane and Pentene, *ACS Catal.*, 3, 1768 (2013).

Alkane Metathesis by Tandem Alkane-Dehydrogenation-Olefin-Metathesis Catalysis and Related Chemistry, *Acc. Chem. Res.*, 45, 947 (2012).

Carbon-Oxygen Bond Activation in Esters by Platinum (0): Cleavage of the Less Reactive, Bond. *Organometallics*, 31, 5018 (2012).

Net Oxidative Addition of C(sp<sup>3</sup>)-F Bonds to Iridium via Initial C-H Bond Activation, *Science*, 332, 1545 (2011).

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C-S Bond Activation of Thioesters Using Pt (0), *Organometallics*, 30, 5147 (2011).

Highly Active and Recyclable Heterogeneous Iridium Pincer Catalysts for Transfer Dehydrogenation of Alkanes, *Adv. Synth. Catal.*, 351, 188 (2009).

There has been growing interest in synthesis and catalytic activity studies of water soluble transition metal complexes in past two decades. Water as a solvent has many potential advantages over organic solvents such as it is environmentally friendly, cheap, and easy to separate from organic products. We are interested to investigate synthesis and catalytic activities of new water soluble transition metal complexes in many catalytic transformation such as reduction of carbon dioxide to formate/formic acid, hydrogenation of ketone, aldehyde and alkene etc. CO<sub>2</sub> hydrogenation to formic acid is not energetically favourable although it is an exothermic reaction due to unfavourable entropy conditions. Water as a solvent will play an important role in this transformation, as it will strongly influence the entropy difference by solvation of both reactants and products.

Concentration of CO<sub>2</sub> in the atmosphere dramatically increased in past few decades due to industrial revolution and growing demand for energy. There has been a great deal of interest to address this issue by utilization of CO<sub>2</sub> as feedstock in recent years due to its non-toxicity, high abundance, and attractive potential for renewable source. However, transformation of CO<sub>2</sub> is challenging due to its high thermodynamic and kinetic stability. We are interested in many different approaches in transformation of CO<sub>2</sub> to useful chemicals. C-H bond

activation and functionalization, catalyzed by transition metal complexes received a great deal of interest in past two decades. Selective transformation of readily available organic compounds to useful organic substrates by functionalization of inert C-H bond has tremendous potential value for synthesis of fine chemicals. Big questions in sp<sup>3</sup> C-H bond activation field still remain to be solved are: 1. Is it limited to few expensive transition metal complexes (e.g. Ir, Rh, Pt etc.)? 2. How to selectively functionalize sp<sup>3</sup> C-H bond to C-O, C-C, C-N, C-X (X= halogen)? 3. How to improve stability, catalytic activity and functional group tolerance (e.g. -CN, -NO<sub>2</sub>, -CO<sub>2</sub>R etc.) of the catalysts? To answer these questions we are interested in developing new synthetic strategies/methodologies for C-H bond activation and functionalization using Ru, Os, Co and Fe catalysts.

Selective and efficient transformation of biomass feedstock to sustainable chemicals and fuels is one of the major focuses in renewable energy to reduce dependence on petroleum based resources. Our research will focus on synthesis of water soluble, thermally robust metal complexes and extensive studies of these complexes for application in biomass and biomass related conversion by hydrogenolysis and deoxygenation.



# Jarugu N. Moorthy



## PROFESSOR

Born in Kotha Kota, Andhra Pradesh, 1964. M.Sc., Bangalore University, 1988; Ph. D., Department of Chemistry, Indian Institute of Science, Bangalore, 1994.

Postdoctoral Fellow, Univ. of Houston, USA, 1994-1995; Univ. of Wuerzburg, Germany, 1995-1996; Univ. of Victoria, Canada, 1996-1998; Asst. Professor, IIT Kharagpur, 1998; Asst. Professor, IIT Kanpur, 1998-2003; Associate Professor, IIT Kanpur, 2003-2007; Professor, IIT Kanpur, 2008-; CRSI Young Chemist of the year, 2004; Ramanna Research Fellowship, 2007-2010; Shanti Swarup Bhatnagar Prize, 2008; Fellow, Indian Academy of Sciences, 2010; Lalit M. Kapoor Chair Professor, 2011-2014; Fellow, Royal Society of Chemistry, 2014.

moorthy@iitk.ac.in, <http://home.iitk.ac.in/~moorthy/>

## Selected References

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Enantioselective Organocatalytic Biginelli Reaction: Dependence of the Catalyst on Sterics, Hydrogen Bonding, and Reinforced Chirality, *J. Org. Chem.*, 76, 396 (2011).

Intramolecular O-H...O Hydrogen Bond-Mediated Reversal in the Partitioning of Conformationally-Restricted Triplet 1,4-Biradicals and Amplification of Diastereo differentiation in their Lifetimes, *J. Am. Chem. Soc.*, 130, 13608 (2008).

A De Novo Design for Functional Amorphous Materials: Synthesis, Thermal and Light Emitting Properties of Twisted Anthracene-Functionalized Bimesitylenes, *J. Am. Chem. Soc.*, 130, 17320 (2008).

Corundum, Diamond, and PtS Metal–Organic Frameworks with a Difference: Self-Assembly of a Unique Pair of 3-Connecting D2d-Symmetric 3,3',5,5'-Tetrakis(4-pyridyl)bimesityl, *Angew. Chem. Int. Ed.*, 44, 2415 (2005).

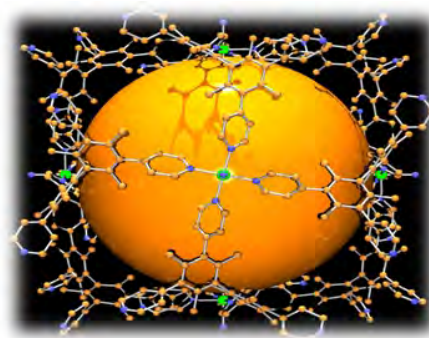
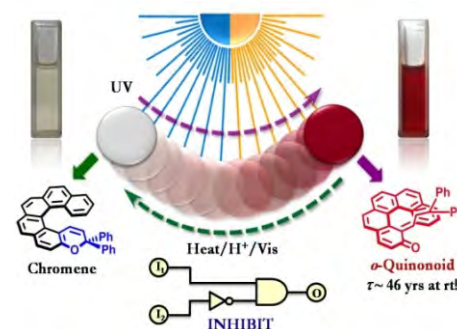
Our research is quite diverse, and it exemplifies the notion that 'structure is an embodiment of reactivity and other attributes such as molecular organization'. The importance of 'structure' bears out in every domain of our research activity, namely, i) organic photochemistry, ii) supramolecular chemistry and iii) mechanistic organic chemistry.

In the area of photochemistry, based on sterics and electronic factors in rationally designed molecules, we endeavor to control the reactivity/phenomenon. The diastereo - differentiating photoreactivity that we have unraveled for ketones with two contiguous stereogenic centers has led to unprecedented insights concerning the well-known Norrish Type II reactions and the behavior of reactive 1,4-biradicals in general. In our recent studies, we have shown how helicity and  $\pi$ -conjugation may modify the photophysical (fluorescence) property and photochromic phenomenon.

In the realm of supramolecular chemistry, our research focus, in addition to the efforts on understanding intermolecular interactions, is centered on controlling molecular ordering by a rational design at the molecular level. In particular, we are intensely pursuing the development of organic functional mimics of inorganic zeolites, i.e., MOFs, for a variety of applications. By exploiting the concepts of supramolecular chemistry in molecular design, we have been focused on developing amorphous organic materials for application in organic light

emitting diodes (OLEDs).

Insofar as mechanistic organic chemistry/organic synthesis is concerned, we have been interested in understanding the reactivity of IBX, o-iodoxybenzoic acid, which has emerged as a remarkable oxidation reagent in the last 15 years. We continue to develop modified IBXs with improved solubility and controlled reactivity. Development of catalytic and chiral IBXs constitutes our present focus.



# Rabindranath Mukherjee



## PROFESSOR

Born in Tribeni, Hooghly, West Bengal, 1953. M. Sc., The University of Burdwan, 1976; Ph. D., The University of Calcutta, 1983.

Junior Research Fellow, IACS, Kolkata, 1978-1983; Post-doctoral Research Associate, IACS, Kolkata, 1983-1985; Harvard University, USA, 1985-1987; IIT Kanpur, 1987-; Director, IISER Kolkata, 2012-; Fellow, Indian Academy of Science, 1999; Fellow, Indian National Science Academy, 2008; Fellow, Royal Society of Chemistry, 2003; Bronze/Silver Medal, CRSI; J. C. Bose National Fellow, DST, 2008; Member, Advisory Board, Dalton Transactions (RSC), 2008-2014; Editorial Board of *Inorganica Chimica Acta* (Elsevier), 2011-2013.

[rnm@iitk.ac.in](mailto:rnm@iitk.ac.in), <http://home.iitk.ac.in/~rnm/>

## Selected References

Neutral, Cationic, and Anionic Low-Spin Iron(III) Complexes Stabilized by Amidophenolate and Iminobenzo-semiquinonate Radical in N, N, O Ligands, *Inorg. Chem.* 53, 36 (2014).

Phenolate- and Acetate (Both  $\mu_2$ -1,1 and  $\mu_2$ -1,3 Modes)-Bridged Linear  $\text{CoII}_3$  and  $\text{CoII}_2\text{MnII}$  Trimers: Magnetostructural Studies, *Inorg. Chem.* 52, 4825 (2013).

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Unprecedented heptacopper(II) cluster with body-centred anti-prismatic topology. Structure, magnetism and density functional study, *Dalton Trans.* 40, 10055 (2011).

Syntheses, X-ray Structures, and Physicochemical Properties of Phenoxo-Bridged Dinuclear Nickel(II) Complexes: Kinetics of Transesterification of 2-Hydroxy-propyl-p-nitrophenylphosphate. *Inorg. Chem.* 48, 7544 (2009).

The Mukherjee Group focuses on systematic development of synthetic coordination chemistry of transition metal ions with designed organic ligands to address diversified research problems. Emphasis is directed to bioinorganic modeling, metal-coordinated ligand radicals, coordination polymers, multi-metal clusters etc.

### Specific research themes include:

(I) Bioinorganic synthetic model work: chemical modeling of tyrosinase and catechol oxidase [dioxxygen activation and aromatic ring hydroxylation, phenoxo-/ hydroxo-bridged dicopper (II) systems]; bio-inspired synthesis of binuclear oxo-/acetate-bridged diiron (III) and dimanganese (III,III; III,IV; IV,IV) systems and reactivity studies of dimanganese(IV) complex with phenols of relevance to photosystem II; demonstration of hydrolysis of biologically-relevant substrates by phenoxo-bridged  $\text{Mn(II)}_2$ ,  $\text{Co(II)}_2$ ,  $\text{Ni(II)}_2$ ,  $\text{Cu(II)}_2$ , and  $\text{Zn(II)}_2$  complexes (detailed kinetic investigations to throw light on the mechanistic aspects); stability and properties of metal-coordinated phenoxyl radical of relevance to galactose oxidase. Low-temperature absorption spectroscopic characterization and reactivity studies of metal- $\text{O}_2$  intermediates.

(ii) Stabilization of nickel(III) and nickel(IV) states; Cobalt-coordinated C-S(thioether) bond cleavage and Co-C bond formation; Stabilization of iron(III)/ruthenium(III)-coordinated o-benzosemiquinonato radical by deprotonated pyridine amide ligands;

Synthesis and properties of ligand-bridged six-coordinate cobalt(III) and four-coordinate cobalt(II) complexes and also a series of hetero-bimetallic complexes; Anion (bisulfate) recognition using ferrocene-appended amide groups; Assembly and properties of a discrete tetrairon(III) cluster and coordination polymers by pyridine amide ligands in their neutral form.

(iii) Metal-coordinated ligand radicals: molecular and electronic structural investigation of metal-coordinated o-iminobenzosemiquinonato anion radical using non-innocent (redox active) ligands and formation of radical-based benzo-triazole ring formation.

(iv) Discovery of a new class of  $\text{Fe(II)N}_6$  spin-equilibria systems, exhibiting interesting cooperativity phenomena (effect of counter-anion and solvate of crystallization).

(v) Co-C bond formation [cobalt(III)-alkyl and cobalt(III)-dialkyl complexes] and investigation of their properties and stabilization of ligand-bridged dinickel(II), dicopper(II), nickel(II)-nickel(I) systems, supported by pyrazole-based chelating ligands.

(vi) Magneto-structural studies of discrete binuclear, trinuclear, and oligonuclear transition metal complexes and coordination polymers.

(vii) Synthesis of half-sandwich organometallic molecules and nucleophilic addition reactions onto the ruthenium(II)-coordinated benzene.

(viii) Identification of non-covalent interactions with emphasis on  $\text{C-H}\cdots\text{Cl}$  hydrogen-bonding.



# Nisanth N. Nair



## ASSOCIATE PROFESSOR

Born at Kallara, Kerala, 1979. M. Sc., Chemistry, IIT Madras, 2001; Ph. D, University of Hannover, Germany, 2004.

Post-doctoral fellow, 2004-2008; Assistant Professor, 2008-2014, IIT Kanpur; Associate Professor, 2014 onwards, IIT Kanpur. Young Scientist Medal, Indian National Science Academy, New Delhi, 2013; Young Associate of the Indian Academy of Sciences, Bangalore, 2012-15; P. K. Kelkar Young Faculty Research Fellow, IIT Kanpur, 2012-15.

[nnair@iitk.ac.in](mailto:nnair@iitk.ac.in), <https://home.iitk.ac.in/~nnair>

## Selected References

Mechanism of Acyl-Enzyme Complex Formation from the Henry-Michaelis Complex of Class C  $\beta$ -Lactamase with  $\beta$ -Lactam Antibiotics, *J. Am. Chem. Soc.*, 135, 14679 (2013).

Hydroxypalladation Precedes Rate Determining Step in the Wacker Oxidation of Ethene, *Chem. Eur. J.*, 19, 4724 (2013).

Rh<sub>1</sub>/  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> Single Atom Catalysis of O<sub>2</sub> Activation and CO Oxidation: Mechanism, Effects of Hydration, Oxidation State and Cluster Size, *Chem. Cat. Chem.*, 5, 1811 (2013)

Thermodynamic and Kinetic Stabilities of Active Site Protonation States of Class C  $\beta$ -Lactamase, *J. Phys. Chem. B* 116, 4741 (2012)

Oxidative Addition of Water to Rh<sub>n</sub> (n=1-4) Clusters on Alumina Surfaces and Spontaneous Formation of H<sub>2</sub>, *J. Phys. Chem. C* 115, 15403 (2011)

Ligand Exchanges and Hydroxypalladation Reactions of the Wacker Process in Aqueous Solution at High Cl<sup>-</sup> Concentration, *J. Phys. Chem. B* 115, 2312 (2011)

I. Development of Theoretical Tools: My group is currently focused on building efficient tools for simulating large-scale catalytic systems and modelling of chemical reactions. Our development work includes designing massively parallel QM/MM code for modelling chemical reactions in zeolites, simulation of metal-organic-frameworks, polymer-composites etc. A new extended Lagrangian approach has been employed to incorporate polarized force-fields within QM/MM, and thus to treat the polarization of MM ions “on-the-fly”. Further development of metadynamics techniques for efficient sampling of chemical reactions in condensed matter system is also a major focus of our research.

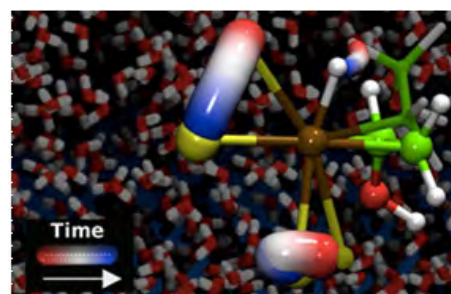
II. Energy: We are interested in computational design of new catalysts for efficient water splitting reactions. In particular, we study Rh/Al<sub>2</sub>O<sub>3</sub> based catalysis for hydrogen evolution from water, and water splitting reactions using Rh/TaON.

III. Health Care: In order to tailor antibiotics with enhanced activity, we are working towards obtaining the molecular details of antibiotic resistance by nosocomial superbugs, including those with the New Delhi Metallo  $\beta$ -lactamase (NDM). By analysing the molecular mechanism of resistance, we hope to come up with novel inhibitors through a bottom-to-top strategy.

IV. Tailored Materials for Advanced Aerospace Applications: In collaboration with the Boeing Company we are trying to understand the thermo-oxidative stability of various polymer materials when exposed to high

temperature. Molecular details of thermo - oxidative reactions are modelled using quantum mechanical calculations, and the reaction kinetics is obtained by micro-kinetic modelling. Through multi-scale modelling, our aim is to come up with novel polymers with a better thermo-oxidative stability and high glass transition temperature.

V: Rh<sub>n</sub>/Y-zeolite Catalysis: Here we explore the molecular details of the hydrogenation reactions of olefins using Rh/Y-zeolite. Dependence of cluster size and partial pressure of hydrogen on the product distribution is studied by the newly developed QM/MM tools.





# Ashis K. Patra



## ASSISTANT PROFESSOR

Born in Durgapur, West Bengal, 1980. M. Sc., The University of Burdwan, 2002; Ph. D., Indian Institute of Science, 2008.

University of Georgia, Athens, Postdoctoral Research Scholar, 2008-2010; Harvard University, Harvard-MIT Division of Health Sciences and Technology, Postdoctoral Research Fellow 2011-2012; IIT Kanpur, Assistant Professor, 2012-.

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## Selected References

Synthesis, properties, and reactivity of a series of non-heme  $\{\text{FeNO}\}^{7/8}$  complexes: Implications for Fe nitroxyl coordination, *J. Inorg. Biochem.*, 118, 115 (2013).

A thermally stable  $\{\text{FeNO}\}^8$  complex: properties and biological reactivity of reduced MNO systems, *Chem. Sci.*, 3, 364 (2012).

Stable Eight-Coordinate Iron(II/III) Complexes, *Inorg. Chem.*, 49, 2032 (2010).

Four-Coordinate As(III)-N,S Complexes: Synthesis, Structure, Properties and Biological Relevance, *Inorg. Chem.*, 49, 2586 (2010).

Synthesis, structure and properties of  $\text{Ni}(\text{N}_2\text{S}_2)$  complexes relevant to Nickel Superoxide Dismutase (Ni-SOD), *Inorg. Chem.*, 48, 5620 (2009).

AT-selective DNA binding and double strand DNA cleavage by copper(II) complexes in PDT window, *Inorg. Chem.*, 48, 2932 (2009).

DNA cleavage in red light promoted by copper(II) complexes of  $\alpha$ -amino acid and photoactive phenanthroline bases, *Dalton Trans.*, 6966 (2008).

Metal-based netropsin mimics showing AT-selective DNA binding and photocleavage activity at red light, *Inorg. Chem.*, 46, 9030 (2007).

My research interests are in the interdisciplinary areas of inorganic chemical biology and bioinorganic chemistry. Our current research goal is to design and study novel cytotoxic metal complexes for targeted therapeutic and diagnostic applications. Currently we are pursuing following research projects in our laboratory.

### I. Therapeutic Applications of Metal Complexes

The biggest change in drug development, particularly in the anticancer field, has been to move towards molecularly targeted agents to circumvent multidrug resistance. This holds promise of more selective and effective drug administration. Transition metals offer beneficial advantages over their more common counterpart of organic drugs. This includes a diverse range of coordination number and stereochemistry, accessible and tunable redox and electronic properties, ligand substitution etc. We are engaged in the development of specifically targeted cytotoxic metal complexes for various therapeutic and diagnostic applications. Their detailed binding interaction studies with biological targets (nucleic acid, proteins etc.) and fate in biological medium were also investigated. Cytotoxicity and mechanism of actions of these metallodrugs will be evaluated to determine their efficacy and mode of actions.

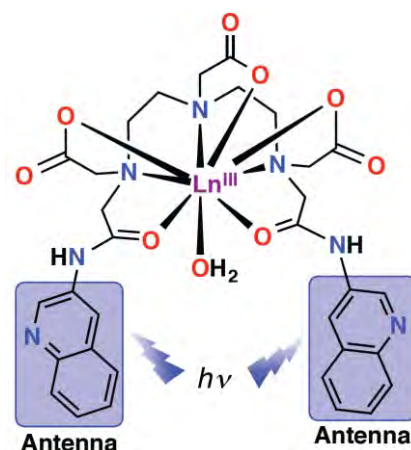
### II. Nitric Oxide Delivery to Biological Targets from Transition Metal Nitrosyl Complexes

This project aims to design and

synthesize transition metal nitrosyl complexes and studying their physicochemical properties and molecular structures. Releasing of nitrosyls from these complexes under various external stimulants will be investigated. We will also study their interaction with potential biological targets (Hb, Mb, GSH etc.) and potential therapeutic applications.

### III. Luminescent Lanthanide Complexes and Biological Applications

Studying chemistry and photophysical properties of lanthanide complexes is an interesting and active research area due to having a wide variety of applications of lanthanide complexes in imaging and diagnostics. Currently we are studying spectroscopic properties, structures and photophysical properties of a series of luminescent lanthanide complexes having organic chromophores as light absorbing antenna molecule for their applications as potential luminescent probes for various analytes or therapeutic applications.



# Dasari L. V. K. Prasad



## ASSISTANT PROFESSOR

Born in Ongole, Andhra Pradesh, 1980. M. Sc., University of Hyderabad, 2002; Ph. D., University of Hyderabad, 2008.

Assistant Professor, Indian Institute of Technology Kanpur, 2013–; NSF Postdoctoral Associate, Cornell University, 2011–2013; Max Planck Society Postdoctoral Research Fellow, MPI-FKF, Stuttgart, 2009–2011; CSIR/DST Senior Research Fellow & Associate, Indian Institute of Science, Bangalore, 2005–2009.

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Silicon Monoxide at 1 atm and Elevated Pressures: Crystalline or Amorphous? *J. Am. Chem. Soc.*, 136, 3410 (2014).

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Synthesis, Crystal Structure and Magnetic Properties of the New One-Dimensional Manganate Cs<sub>3</sub>Mn<sub>2</sub>O<sub>4</sub>, *J. Am. Chem. Soc.*, 134, 11734 (2012).

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Stuffed fullerene-like boron carbide nanoclusters, *Appl. Phys. Lett.* 96, 023108 (2010).

Stuffing improves the stability of fullerene like boron clusters, *Phys. Rev. Lett.* 100, 165504 (2008).

Electronic structure and bonding of beta-rhombohedral boron using cluster fragment approach, *Phys. Rev. B* 72, 195102 (2005).

Our research focus is to understand and predict the electronic structure and properties of materials under ambient to extreme conditions of high temperature and pressure using approximate theoretical quantum mechanical calculations and chemical intuition. The properties of interest range from chemical bonds to superconductivity. Establishing common threads between the chemistry and physics of materials of interest is one of our emphases.

Chemical and physical properties of a chemical constituent in any state, be it gas, liquid, solid, depend upon its atomic and electronic structure. It is of utmost priority, therefore, to have knowledge of its structure, not only to understand the experimental/theoretical outcomes but also to improve and predict the properties, and design viable novel materials with desired properties. All in all, the structure of matter is the holy grail of the chemistry and physics of materials. It is generally possible to predict the structure of a given chemical composition (gas-phase molecule or crystalline solid) using wavefunction/density functional theoretical calculations coupled with evolutionary or stochastic structure prediction algorithms.

$$E = \min_{\Psi} \langle \Psi | \hat{T} + \hat{V}_{ee} + \hat{V} | \Psi \rangle$$

We seek to apply and develop novel theoretical algorithms/models in predicting crystal structures.

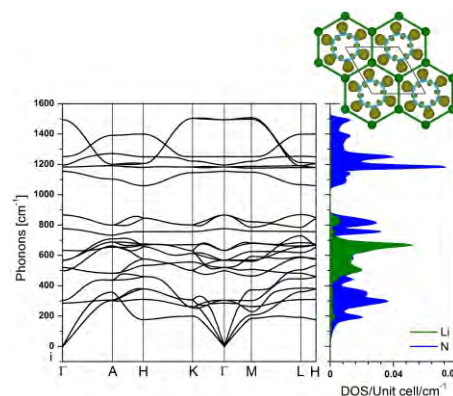
Our studies are also aimed at

investigating the mechanistic pathways in solid-state structural phase transitions – bond breaking and bond forming in solids, reconstructive, displacive, and order-disorder phase transitions. We are interested in developing theories and computational algorithms to understand the mechanism of atomistic resolution details in solid-state structural phase transitions.

One of our long term goals is to design a room-temperature superconducting material, in particular, we are working on low-Z systems within the BCS phonon mediated superconducting mechanism,

$$\lambda = 2 \int_0^{\infty} \frac{\alpha^2 F(\omega)}{\omega} d\omega$$

In a nutshell our research priorities include the study of electronic structure of materials, phase transitions in complex solids, and superconductivity in low-Z solid state materials.





# Gurunath Ramanathan



## PROFESSOR

Born in New Delhi, 1966. M. Sc., (Chem), Delhi University, 1988; Ph. D., Indian Institute of Science (IISc), Bangalore, INDIA, 1994.

Post docs at MIT, Cambridge, USA, 1995-1996; Karolinska Institutet, Stockholm, Sweden, 1996-1999; Sveriges Lantbruks Universitet, Uppsala, Sweden 1999-2000; Assistant Professor, IIT Kanpur 2000-2007; Associate Professor, IIT Kanpur, 2008-2011; Professor, IIT Kanpur, 2011-; Axel Wenner-Gren Foundation Fellow, 1998.

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## Selected References

Biomining of 3-nitrotoluene by diaphorobacter species, Biodegradation, 24, 645 (2013)

Integrated sorting, concentration and real time PCR based detection system for sensitive detection of microorganisms, Sci. Rep. 3, 3266 (2013)

Segregation into chiral enantiomeric conformations of an achiral molecule by concomitant polymorphism, Cryst. Growth Des., 12, 1823 (2012)

Excited state relaxation dynamics of model green fluorescent protein chromophore analogs: evidence for cis-trans isomerism, J. Phys. Chem. A, 115, 13733 (2011).

A change in the  $310\text{-}$  to  $\alpha\text{-}$  helical transition point in the heptapeptides containing sulfur and selenium, Cryst. Growth Des., 11, 2238 (2011)

Biomining of N,N-Dimethylformamide by paracoccus sp. Strain DMF J. Hazard. Mater., 171, 268-272 (2009)

A patent on an improved organic optoelectronic device has been granted at Delhi, Ref. No., 3263/RQ – DEL 2007

Proteins perform a variety of cellular functions. We study protein function using peptide or organic molecules as models. With our broad interest in peptides we are trying to mimic the function of complex proteins through rational design. For this, we use non-protein synthetic amino acids as scaffolds to tailor the peptides to get secondary structure folds to address fundamental aspects of protein folding. Our findings reveal that the interaction of side chains with the main chain directs the structure of these molecules both in solution and in solid state. This research led us to the successful use of green fluorescent protein chromophore models in organic solar cells.

We are actively involved in isolation of microbes from various environments that specifically target and degrade organic pollutants. In this journey, we recently reported the diaphorobacter species strain DS-2 that degrades 3-nitrotoluene (isolated from an industrial waste treatment plant) and paracoccus strain DMF that completely degrades dimethylformamide (isolated from domestic waste water) and the complete biochemical pathway of degradation of pollutants in these strains was determined. The first degradative enzyme (3-nitrotoluene dioxygenase) from diaphorobacter species strain DS-2 which preferentially transforms only 3-nitrotoluene to a mixture of 3- and 4-methyl catechols was also cloned by us.

This complex protein is a mononuclear iron containing enzyme that has a Rieske  $2\text{Fe-2S}$  iron-sulfur cluster. It contains

two oxygenase subunits (small  $\alpha$ -23 kDa and large  $\beta$ -50 kDa), one reductase subunit (35 kDa) and a ferredoxin subunit (12 kDa). The structure of the complete oxygenase subunits using its homology with a known dioxygenase (nitrobenzene dioxygenase) has been modeled by us (see figure below).

In collaboration, we have recently developed a sensitive detection of microorganisms comprising of an integration of techniques like cell sorting, selective concentration and on-chip real time PCR.



Homology modeled oxygenase from diaphorobacter sp. strain DS-2. The large ( $\alpha$ -chain turquoise) and small ( $\beta$ -chain green) of 3-nitrotoluenedioxygenase superposed on the protein nitrobenzene dioxygenase from *Comamonas* sp. JS765. The Rieske iron is circled and the mononuclear iron is shown in the square.



# Ramesh Ramapanicker



## ASSISTANT PROFESSOR

Born in Vechoor, Kerala, India, 1978. M. Sc., Mahatma Gandhi University, 2001; Ph. D., Indian Institute of Science, 2007.

Uppsala University, Postdoctoral researcher, 2007-2010; Assistant Professor, Department of Chemistry, Indian Institute of Technology Kanpur, 2010-.

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## Selected References

Unusual reactions of the 1,3-dithiane derivative of the Garner aldehyde and related compounds, *Synthesis*, 45, 1997 (2013).

Powerful binders for the D-dimer by conjugation of the GPRP peptide to polypeptides from a designed set-illustrating a general route to new binders for proteins, *Bioconjugate Chem.*, 24, 17 (2013).

Synthesis of  $\gamma$ -oxo  $\gamma$ -aryl and  $\gamma$ -aryl  $\alpha$ -amino acids from aromatic aldehydes and serine, *Eur. J. Org. Chem.*, 36, 7120 (2012).

Mixed pentafluorophenyl and *o*-fluorophenyl esters of aliphatic dicarboxylic acids: efficient tools for peptide and protein conjugation, *RSC Advances*, 2, 908 (2012).

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Powerful protein binders from designed polypeptides and small organic molecules-A general concept for protein recognition, *Angew. Chem. Int. Ed.* 50, 1823 (2011).

An improved procedure for the synthesis of dehydroamino acids and dehydropeptides from the carbonate derivatives of serine and threonine using tetrabutylammonium fluoride, *J. Pept. Sci.* 16, 123 (2010).

Propargyl Chloroformate. *Encyclopedia of Reagents for Organic Synthesis*, John Wiley and Sons. DOI: 10.1002/047084289X.rn00816

Organic Synthesis: Chiral synthons (chirons) derived from natural amino acids and sugars are employed in the synthesis of unusual amino acids, carbohydrate derivatives and natural products. Asymmetric transformations of these chirons provide an opportunity to target molecules containing multiple and contiguous stereogenic centres. We use asymmetric organocatalytic reactions such as proline catalyzed  $\alpha$ -amination and  $\alpha$ -hydroxylation to synthesize highly functionalized targets in very high diastereo- and enantiopurity.

Unusual amino acids in peptide design: The use of unusual amino acids in peptides to impart directed hydrogen bonding is an effective tool to get oligopeptides with desired secondary structures. Such structures can not only provide basic understanding of protein folding, but can also be used to synthesize peptides that may self-assemble and be used for drug delivery and related applications.

We are involved in the synthesis and application of amino acids containing hydrogen bond donor and acceptor side chains that are designed to stabilize helices and turns in smaller peptides. Substituted proline derivatives are designed to enhance cis/trans peptide bonds and to stabilize specific turns in peptides containing them.

The synthesis of C-linked organometallic and fluorescent amino acids for sensor applications is another area that we actively pursue.

Peptide Conjugates: Functionalizing peptides with small molecules that are biologically active is an efficient method for generating molecules with

the potential to be used in therapeutic and diagnostic applications.

We are involved in the synthesis of peptides conjugated with nucleophilic molecules to be used for the reactivation of acetylcholine esterase, rendered inactive by exposure to organophosphorous compounds. Using a similar approach, we are also attempting to develop molecular sensors for organophosphorous and related chemical warfare agents.

We are developing small molecule conjugates of peptides to be used for glycosidase inhibition and cancer chemotherapeutics.

# Madhav Ranganathan



## ASSISTANT PROFESSOR

Born in Chennai, India, 1974. M.Sc., IIT Bombay, 1996; Ph.D, Stanford University, 2003.

University of Maryland, College Park, USA. 2003-2006; CNRS, Marseille, France, 2006-2007; IIT Kanpur, 2007-.

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Submonolayer growth study using a solid-on-solid model for  $2 \times 1$  reconstructed surfaces of diamond-like lattices, *Surf. Sci.*, 630, 174 (2014)

Impurity Effects in Crystal growth from solutions: Steady states, transients and step bunch motion, *J. Cryst. Growth.*, 393, 35 (2014).

A genome-wide screen indicates correlation between differentiation and expression of metabolism related genes, *PLoS ONE* 8, e63670, (2013).

Impurity induced step pinning and recovery in crystal growth from solutions, *Phys. Rev. Lett.*, 110, 055503 (2013).

Kinetic Monte Carlo simulations of heteroepitaxial growth with an atomistic model of elasticity, *Surf. Sci.*, 606, 1450 (2012).

Spiral Evolution in Confined Geometry, *Phys. Rev. Lett.*, 95, 225505 (2005).

Understanding the morphology of growing crystals under different conditions is a fundamental problem that has implications in a wide variety of systems like electronic and optoelectronic devices and biological systems like kidney stone growth and abalone shell growth.

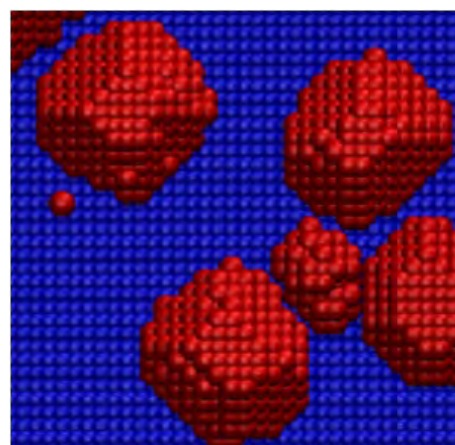
Over the years our group has been using techniques from nonequilibrium statistical mechanics and computer simulation to address different aspects of this problem.

One major area where we are actively working in is heteroepitaxy, wherein a crystalline film is grown on a crystalline substrate of a different material. The difference in the two materials leads to a strain in the growing film that can lead to a change in the nature of the growing surface. A very well-studied example of such a system is the Germanium on Silicon(001) surface. Experiments have revealed that the growth of the Ge film is flat for the first three atomic layers but becomes mounded for layers after that. The size and shapes of the mounds have been characterized experimentally and several theoretical approaches have been proposed to explain the growth features. To address this problem, we adopt the technique of lattice-based kinetic Monte Carlo simulations with explicit elastic effects. Through our calculations we have investigated the interplay between the inherent anisotropy in the surface energy of the Ge film and the strain effects due to the mismatch with the substrate.

In addition to the Silicon-Germanium system, we are also looking at Gallium Nitride based systems using similar

lattice-based kinetic Monte Carlo simulations. In this case, there are additional complexities due to the multiple species involved in the growth process. Further, we have also worked on crystal growth from impure solutions wherein impurities can completely stop growth, even when the solution is supersaturated in the growing species. We model the process of crystal growth via the motion of surface steps and show how impurities can cause step-bunching, step-pinning and the coherent motion of step bunches.

Another area where we are actively working is in problems in bioinformatics and biophysical chemistry. Our work included statistical analysis of Genetic expression information at multiple time-stages and the analysis of transport of Calcium across the neuronal cells.





## PROFESSOR

Born in Narasaraopet, A. P., 1966. M. Sc. (Org. Chem.), Nagarjuna University, 1988; M. Phil., University of Hyderabad, 1990; Ph. D., University of Hyderabad, 1996.

PostDoc at NIMC, NIAR and AIST, Tsukuba, JAPAN, 1997-2002; University of North Carolina (UNC) Chapel Hill, USA, 2002-2003; Assistant Professor, IIT Kanpur 2003-2007; Associate Professor, IIT Kanpur, 2008-2011; Professor, IIT Kanpur, 2011-; CREST Fellow (JST, JAPAN), 1997-2000.

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Pd-catalyzed chemoselective threefold cross-coupling of triarylbismuths with benzylic bromides,  
RSC Advances, 13, 6794 (2013)

Pd-Catalyzed Tandem Chemo-selective Synthesis of 2-Arylbenzo-furans using Threefold Arylating Triarylbismuth Reagents, Eur. J. Org. Chem., 781 (2013)

Pd-catalyzed threefold arylations of mono, di and tetra-bromoquinones using triarylbismuth reagents,  
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Transition-metal catalyzed C-C bond formation using organobismuth compounds, Top. Curr. Chem., 311, 199 (2012)

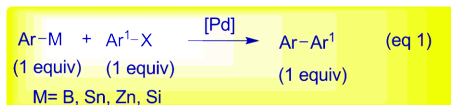
Synthesis of functionalized 2-aryl-thiophenes with triarylbismutorganometallic nucleophiles under palladium catalysis, Syn. Lett., 1324 (2011)

Pd(o)-catalyzed couplings using bromide and chloride derivatives of Baylis-Hillman adducts with triarylbismuths as atom-efficient multi-coupling nucleophiles, Tetrahedron, 66, 3623 (2010)

Pd-catalyzed domino synthesis of internal alkynes using triarylbismuths as multicoupling organometallic nucleophiles, Org. Lett., 12, 2048 (2010)

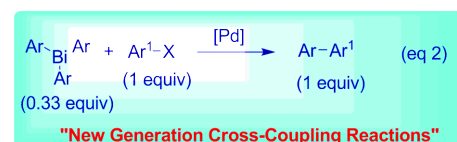
Our primary research revolves around the 'development of green organometallic reagents and their applications to organic synthesis'. We embarked upon the development of 'new generation cross-coupling reactions' using triarylbismuths as 3-fold coupling reagents. Over the years, we have developed a variety of new coupling reactions using organobismuth chemistry, with a diverse range of reactivity under palladium catalyzed conditions with high atom-economy. Further research activities in our group include convergent organic synthesis, microwave mediated organic synthesis, auto-catalysis, metal catalyzed reactions and other reactions of contemporary interest.

New Generation Green Cross-Coupling Reactions: Cross-coupling methods have enriched the art of organic synthesis and evolved as effective synthetic tools to construct complex molecular systems. The well-known coupling reactions such as Suzuki, Stille, Negishi, etc. invariably involve only one C-C bond formation (eq. 1).



We envisaged that a paradigm shift in the reagent capability is necessary to make these reactions more green and atom-economic with additional potential for multi C-C couplings in one-pot operation.

Triarylbismuths, which are non-toxic, air stable, and contain three aryl groups (e.g., Figure 1), appeared to us as the most promising green organometallic reagents with 3-fold coupling capabilities (eq. 2).



These reagents could, in principle, be employed in sub-stoichiometric 1/3 molar equivalents with increased atom-efficiency in a one-pot operation (eq. 2 vs eq. 1). Our consistent efforts have led to the development of new generation cross-coupling reactions with triarylbismuths reagents, and opened up a plethora of new opportunities in terms of reactivity and selectivity. Thus, a new series of Pd-catalyzed coupling reactions have been developed involving aryl, heteroaryl, acyl, allyl and vinyl couplings, bis-couplings, carbonylations and domino one-pot coupling reactions.

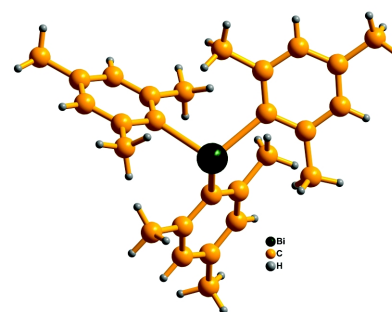


Figure 1. The Structure of trimesitylbismuthine.



# Sankar P. Rath



## PROFESSOR

Born in Midnapur, West Bengal, 1972. M. Sc., Calcutta University, 1994; Ph. D., IACS, Kolkata, 1999.

NIH Post-doctoral Research Associate at University of California, Davis, USA, 2000-2004; Assistant Professor at IIT Kanpur, 2004-2009; Associate Professor at IIT Kanpur, 2010-2013; Professor at IIT Kanpur, 2014-. Alexandervon Humboldt Research Fellowship for Experienced Researchers, 2012; P. K. Kelkar Young Faculty Research Fellowship, 2009-2012; CRSI Bronze medal, 2014.

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Hydrogen Bonding Interactions Trigger a Spin Flip in Fe(III) Porphyrin Complexes, *Angew. Chem. Int. Ed.*, 54, 4796 (2015)

Step-wise Induction, Amplification and Inversion of Molecular Chirality Through the Coordination of Chiral Diamines with Zn(II)bisporphyrin, *Chem. Commun.*, 51, 895 (2015).

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Protonation of an oxo-Bridged Diiron Unit Makes Two Iron Centers Different: A New Class of Diiron(III)- $\mu$ -hydroxo Bisporphyrin and Control of Spins by Counter Anions, *Chem. Eur. J.*, 18, 13025 (2012).

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A Remarkably Bent Diiron(III)- $\mu$ -Hydroxo Bisporphyrin: Unusual Stabilization of Two Spin States of Iron in a Single Molecular Framework, *J. Am. Chem. Soc.*, 132, 17983 (2010).

Rath's group at IIT Kanpur is engaged studying a wide range of bioinorganic and biological systems, all of which fall under the general theme of gaining a better understanding of the heme centers in heme proteins that are vital to the life of almost all living organisms. The group is currently engaged in several broad research areas such as:

### Unfolding Mystery of Multi-Heme Cytochromes

Multiheme cytochromes c constitutes a widespread class of proteins with essential functions in electron transfer and enzymatic catalysis. Understanding the significance of these motifs is crucial for the elucidation of the highly optimized properties of multiheme cytochromes c.

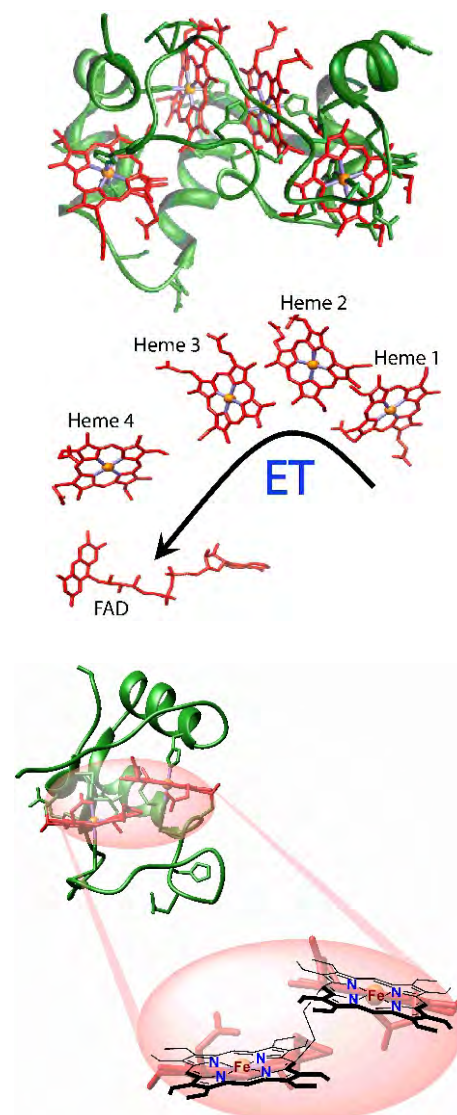
### Probing Molecular Chirality using Metallo-Bisporphyrin Hosts with Exciton Coupled Circular Dichroism (ECCD)

The relative orientation of two chromophores in space in a chiral host-guest complex results in a bisignate CD curve with two bands of opposite sign and similar intensity in the porphyrin spectral regions which is diagnostic of the guest's absolute configuration.

### Light Induced Electron/Energy Transfer

One of the problems to be solved was the role of 'special pair' in photosynthesis which is being investigated extensively. The Rath's group has been using extensively a wide variety of spectroscopic techniques including X-ray diffraction study, variable

temperature magnetic, NMR, EPR and Mössbauer spectroscopy and also DFT for structure-function correlation. The progress of the reactions are monitored in situ in solution along with the structural elucidation utilizing paramagnetic NMR spectroscopic technique.



# Manogaran Sadasivam



## PROFESSOR

Born in Tamil Nadu, 1954. M. Sc., Madras University, 1976; Ph. D., Indian Institute of Science, Bangalore, 1982.

Post-doctoral Research Associate, NIH Resource for NMR, Syracuse University, New York, 1983-1984; Research Specialis, University of California, San Francisco, 1984-1987; Indian Institute of Technology Kanpur, 1987-; Visiting Professor, Department of Applied Chemistry, Tohoku University, Sendai, Japan, 2003; Fulbright-Nehru Senior Research Fellow, 2010-2011.

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Vibrational spectra of adamantanes  $X_{10}H_{16}$  and diamantanes  $X_{14}H_{20}$  ( $X=C, Si, Ge, Sn$ ): A theoretical study,  
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Force field calculation of molecules in isotopomers of different symmetries in vibrational analysis,  
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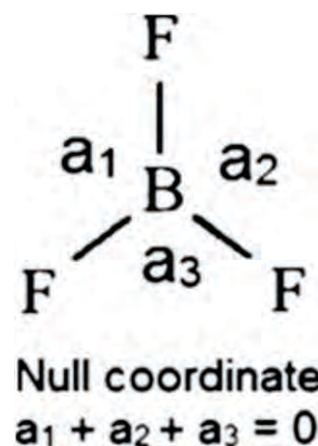
Interpretation and accurate prediction of vibrational spectra- a modified ab initio scaled quantum mechanical approach,  
Theochem, 432, 139 (1998)

We are interested in understanding the molecular force fields and potential energy surface. We use ab initio and DFT methods to study the structure, bonding and molecular vibrations. The force fields obtained by these methods on the optimized geometries of molecules are used to study the harmonic force fields in terms of force and compliance constants by performing normal mode analysis (NMA). A software is being developed locally for this purpose based on the QCPE program UMAT(#576). Several innovative ideas described in our publications for doing NMA are incorporated in this program to achieve the goal of automated vibrational analysis. The concept of orthogonal transformation, different scaling algorithms including scaled quantum mechanical (SQM) approach, determination of unique force constants for isotopomers of different symmetries, compliance constants in internal coordinates are some of the features available in the program.

Since the real molecular potential is anharmonic, understanding the anharmonicity effects are important. For this purpose evaluations of symmetry unique cubic and quartic force constants, anharmonicity constants, Fermi resonance and vibration-rotation interaction constants of molecules are necessary. Work is in progress in this direction. Molecular symmetry is used to reduce the labour as much as possible. Infrared and Raman spectral intensities play a crucial role in understanding the

electronic structure of molecules in terms of the derivatives of dipole moment and polarizability. This is another area of interest which is being explored

The computed force and compliance constants are used to quantify the aromaticity, ionization constants and to explain the vibrational spectral features.



# Narayanasami Sathyamurthy



## PROFESSOR

Born in Sethur, Tamilnadu, India, 1951. M. Sc., Annamalai University, 1972; Ph. D., Oklahoma State University, USA, 1975.

Post-doc, University of Toronto, Canada, 1975-78; Lecturer/Asst.Professor/Professor/Institute Chair Professor, IIT Kanpur, 1978-; Alexander von Humboldt Fellow, Max-Planck-Institut f. Strömungsforschung, Göttingen, Germany, 1986-87; Shanti Swarup Bhatnagar Prize, CSIR, 1990; Fellow, Indian Academy of Sciences, 1990; Fellow, Indian National Science Academy, 1992; Fellow, Third World Academy of Sciences, Trieste, Italy 2005; J. C. Bose National Fellow, 2007-; IIT Kanpur Fellow, 2013; Director IISER Mohali, 2007-.

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Interpretation of the accidental predissociation of the  $E_1\Pi$  state of CO, J. Chem. Phys., 140, 164303 (2014).

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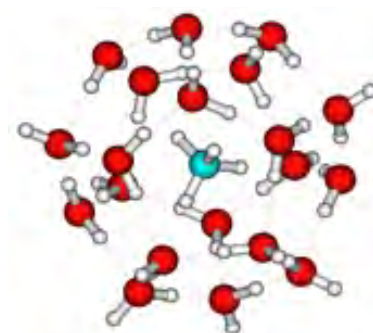
Professor Sathyamurthy's research interest has been investigations in the area of molecular reaction dynamics, using quasiclassical trajectory calculations and time-dependent quantum mechanical methods as tools. Starting from ab initio calculations of the potential energy surface and fitting an analytic function to the ab initio data and using the potential energy surface to compute state-to-state reaction cross section and other observables for elementary chemical reactions has been the major activity of the group. The group had focussed special attention on the dynamics of  $\text{He} + \text{H}_2^+ \rightarrow \text{HeH}^+ + \text{H}$  reaction and the isotopic branching in  $\text{He}, \text{HD}^+$  collisions. Recently, they have reported the results of a three dimensional quantum mechanical study of the collision induced dissociation process too. In all cases, the computed results have been compared with the best available experimental results. Perhaps, one of the best ab initio potential energy surfaces for the  $\text{H}_3^-$  system comes from the group.

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

Determining accurate ab initio potential energy curves for the ground and excited states of anionic species is a

challenging task. This is particularly so because of the curve crossing between the anionic and neutral species and the resulting autoionization. The group has computed reliable ab initio potential energy curves for  $\text{H}_2^-$ ,  $\text{CH}^-$ ,  $\text{NH}^-$  and  $\text{OH}^-$ . They have paid special attention to the study of the ground and excited electronic states of isoelectronic species to understand the relation between the neutral and the anionic species.

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





# Pratik Sen

## ASSOCIATE PROFESSOR

Born in Suri, West Bengal, India, 1977. M. Sc., Visva-Bharathi University, 2001; Ph. D., Indian Association for the Cultivation of Science, India, 2006.

PostDoc., RIKEN, Japan, 2006-2008; Assistant Professor, IIT Kanpur, 2008-2014; Associate Professor, IIT Kanpur, 2014-; JSPS Fellow, 2006-2008; Young Scientist Medal, Indian National Science Academy, New Delhi, 2013.

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Mechanistic investigation of domain specific unfolding of human serum albumin and the effect of sucrose, *Protein Sci.*, 22, 1571 (2013).

Spectroscopic evidence of the presence of an activation barrier in the otherwise barrierless excited state potential energy surface of auramine-O: A femtosecond fluorescence up-conversion study, *J. Chem. Phys.*, 139, 124302 (2013).

Dielectric Controlled Excited State Relaxation Pathways of a Representative Push-Pull Stilbene: A Mechanistic Study using Femtosecond Fluorescence Up-conversion Technique, *J. Chem. Phys.*, 138, 084308 (2013).

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Femtosecond Excited State Dynamics of 4-Nitrophenyl Pyrrolidinemethanol: Evidence of Twisted Intramolecular Charge Transfer and Intersystem Crossing involving Nitro Group, *J. Phys. Chem. A*, 115, 8335 (2011).

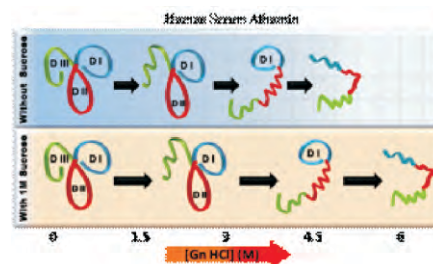
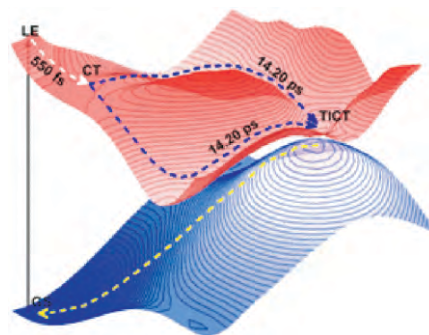
The central approach of this laboratory is the mechanistic investigation of photo-induced processes of important organic and inorganic molecules in real time. Primarily we are devoted to investigate the excited state characteristics of broad range of molecules in the time scale ranging from femtoseconds to nanoseconds. The brief fields of interest include the dynamics of biological macromolecules like proteins, DNA, etc., the excited state ultrafast dynamics of many novel chromophores like fluorescent protein chromophore analogs, metal complexes, etc. Effect of nano-confinement and heterogenous media also share one of the prime locus of research in the laboratory. The main aim is to interpret natural observation and to gain complete knowledge of system property from the knowledge of excited state relaxation dynamics. In addition we are as well commencing the non-linear laser spectroscopic study of liquid-air and solid-air interfaces.

Our laboratory is equipped with

1. Femtosecond transient absorption spectrometer
2. Femtosecond fluorescence up-conversion spectrometer
3. Picosecond TCSPC system
4. Steady state fluorimeter
5. Spectrophotometer
6. Home built fluorescence correlation spectrometer etc.

Our group have studied the ultrafast excited state relaxation dynamics of important NLO dye to trace the relaxation pathways and connected to its properties. This work became one of

the most read articles in The Journal of Physical Chemistry A. We also have confirmed the role of protein scaffold in reducing the non-radiative pathways, leading to highly luminescent nature of wild type GFP by studying GFP chromophore analogs. Using ultrafast laser spectroscopy, we also have measured the microviscosity of water trapped in AOT reverse-micelle to explore the possibility of using ultrafast dynamics to understand the system property.



# Anand Singh



## ASSISTANT PROFESSOR

Born in Gorakhpur, UP, 1981. M. Sc., Indian Institute of Technology Bombay, 2004; Ph. D., Vanderbilt University, 2009.

Postdoctoral Associate, Sanford-Burnham Medical Research Institute at Lake Nona, Orlando-FL, U.S.A., 2009-2012; IIT Kanpur, 2013-.

[anands@iitk.ac.in](mailto:anands@iitk.ac.in), <http://home.iitk.ac.in/~anands/>

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Synthesis of OxindolylPyrazolines and 3-Amino Oxindole Building Blocks via a Nitrile Imine [3+2] Cycloaddition Strategy, *Org. Lett.*, 14, 5266 (2012).

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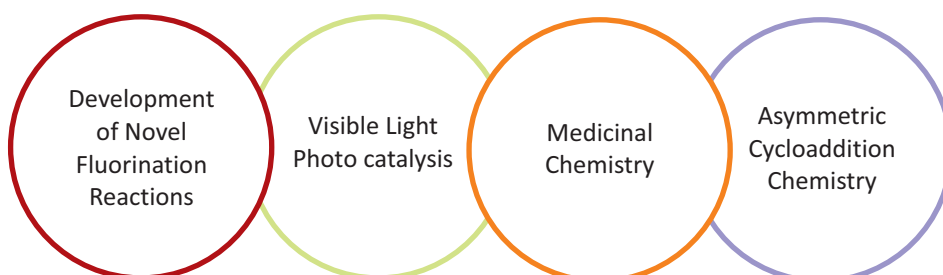
A Diastereo- and Enantioselective Synthesis of  $\alpha$ -Substituted syn- $\alpha,\beta$ -Diamino Acids, *J. Am. Chem. Soc.*, 130, 5866 (2008). (Highlighted in *Syn. facts* 2008, 7, 0757).

Chiral Proton Catalysis: Enantioselective Brønsted Acid Catalyzed Additions of Nitroacetic Derivatives as Glycine Equivalents, *J. Am. Chem. Soc.*, 129, 3466 (2007).

Our recently established research group at IITK has research interests broadly encompassing the areas of enantioselective catalysis, development of new reactions, and medicinal chemistry.

The unifying theme of our research is the development of new and efficient chemical transformations in order to create novel small molecule organics for potential applications in the fields of medicine, material science, and agrochemicals. One of our programs focuses on the development of novel fluorination reactions. Owing to the important applications of fluorinated compounds as drugs, diagnostic tools (PET imaging), and as agrochemicals, the synthesis of such molecules is of contemporary interest, and our lab is exploring the synthesis of novel fluorinated small molecules by developing fluorination strategies that employ fluoride anion as the source of fluorine. In addition to expanding the fluorinated chemical space, this strategy will lead to a more economical approach toward fluorinated compounds as opposed to the vast majority of current methods that employ electrophilic fluorination reagents.

A second area of research in our laboratory is photoredox catalysis wherein we aim to develop visible-light mediated reactions. Visible light represents an abundant, inexpensive, and clean source of energy and through its synergistic use with a suitable catalyst, it has been possible to activate certain types of organic molecules toward interesting, novel, and useful reactions. We are investigating a variety of olefin functionalization and cyclization reactions that will result in novel scaffolds that are valuable synthetic intermediates and also represent novel chemical spaces relevant to drug discovery and chemical biology.



# Vinod K. Singh



## PROFESSOR

Born in Azamgarh, UP, 1959. M. Sc., Banaras Hindu University, 1980; Ph. D., M. S. University Baroda (Mali-Chem Research Centre, Nandesari), 1986; D. Sc (hc).

Postdoctoral: University of Calgary, Canada, 1985-1986; University of British Columbia, Canada, 1986-1987; Harvard University (Advisor: Prof. E. J. Corey), USA, 1987-1990. Member, Scientific Advisory Council to the Prime Minister (SAC to PM); Founder Director, Indian Institute of Science Education and Research, Bhopal, 2008; Swarnajayanti Fellowship, 1998; Shanti Swarup Bhatnagar Prize, 2004; Goyal Prize, 2011; Fellow, Indian National Science Academy, 2011; Distinguished Alumnus Award, BHU, 2012; Padma Shri, 2014.

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Asymmetric Alkynylation/Lactamization Cascade: An Expeditious Entry to Enantiomerically Enriched Isoindolinones *Angew. Chem. Int. Ed.*, 53, 10737 (2014).

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Highly Enantioselective Friedel-Crafts Reaction of Indoles with 2-Enoylpyridine 1-Oxides Catalyzed by Chiral Pyridine 2,6-Bis (5',5'-diphenyloxazoline)-Cu(II) Complexes, *Org. Lett.*, 10, 4121 (2008).

Professor Singh's research work falls in the area of synthetic organic chemistry, more specifically, asymmetric synthesis. Prof. Singh has accomplished total synthesis of several bioactive natural products and medicinally important compounds and had developed a number of novel asymmetric methodologies for the synthesis of several optically pure and therapeutically as well as pharmacologically useful chiral building blocks of immense synthetic importance.

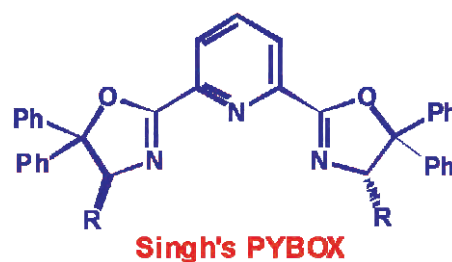
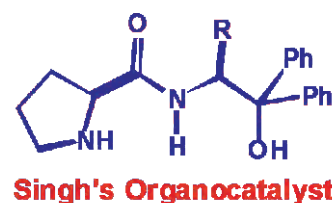
His initial research in the area of asymmetric synthesis particularly on enantioselective deprotonation of epoxides and allylic oxidation of olefins, received high appreciation from world all over.

Currently, Prof. Singh is working in the area of Asymmetric Catalysis, which is one of the most important and cutting-edge area of research in Synthetic Chemistry. Towards the metal-catalyzed enantioselective transformations, his group has successfully applied *i*Pr-Pybox-diPh ligands in enantioselective allylic oxidation of olefins and enantioselective propargylation reactions.

In 2008, the group explored bidentate chelating substrate 2-enoylpyridine N-oxide as a new template in asymmetric Michael reactions. Using this template they carried out enantioselective Michael reactions of indoles, pyrroles, dialkyl malonates, 4-hydroxy coumarins, and 1,3-dicarbonyls and Mukaiyama-Michael reaction as well using silylenolethers thus expanding the scope of *i*Pr-Pybox-diPh ligands.

In 2006, Singh and his research group

designed a new organocatalyst, popularly known as Singh's catalyst for asymmetric Aldol reaction. This is one of the best catalysts known for enantioselective aldol reactions till date. Another area where Singh's group contributed significantly is the enantioselective organocatalytic reactions using H-bonding catalysts via dual activation mode.





# Basker Sundararaju



## ASSISTANT PROFESSOR

Born in Mettupalayam, Tamilnadu, 1980. M. S., Universite de Rennes, France, 2008; Ph. D., Universite de Rennes, France, 2011.

Max-Planck Group post doctoral fellow, 2011 – 2012; Alexander Von Humboldt Fellow, 2012 – 2013; Assistant Professor, Indian Institute of Technology Kanpur, 2013-.

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## Selected References

A *Trans*-Selective Hydroboration of Internal Alkynes, *Angew. Chem. Int. Ed.*, 52, 14050 (2013).

A Functional Group Tolerant *Trans*-Hydrogenation of Alkynes, *Angew. Chem. Int. Ed.*, 52, 355 (2013).

Selective Carbon-Carbon Bond Formation: Terpenylation Of Amines Involving Hydrogen Transfer, *Green. Chem.*, 15, 775 (2013).

Transition Metal Catalyzed Nucleophilic Allylic Substitution: Activation of Allylic Alcohols via  $\pi$ -Allyl Species, *Chem. Soc. Rev.*, 41, 4467 (2012).

Isoquinoline Derivatives via Stepwise  $Sp^2$  and  $Sp^3$  C-H bond functionalization, *J. Org. Chem.*, 77, 3674 (2012).

Ruthenium Catalyzed Reductive Amination Of Allylic Alcohols, *Org. Lett.*, 13, 3964 (2011).

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Light Driven Hydrogen Generation: Efficient Iron Based Water Reduction Catalysts, *Angew. Chem. Int. Ed.*, 48, 9962 (2009).

Catalysis, the science of accelerating chemical transformations developed significantly in the last few decades and still continues to attract the attention of chemists for its major contribution in the synthesis of more complex molecules in fewer steps. In a relative term, we strongly believe that without catalysts and catalytic technologies, the access to all of the materials needed for our daily lives would not be possible or suffer in quality.

Having said that till today, many chemical reactions was carried out through classical organic synthesis, which includes selective functionalization such as nitration; halogenation, cyanation, etc. often generate several tons of hazardous waste. With these facts, there is a need for most innovative and versatile catalytic methods for environmentally sustainable process. In particular, the goal of sustainable process is to develop technologies that use fewer raw materials and less energy, which maximize the use of renewable resources, and minimize or eliminate the use of hazardous chemicals. Of late, it's well known that organometallic chemistry plays a vital role in the development of green and sustainable environment, one of the important features of catalysis.

In light of these requirements, our research program concentrates on transition metals as a means of achieving efficient catalytic system for activation of carbon-hydrogen, carbon-carbon and carbon heteroatom. By understanding the reaction processes, ligand properties and their coordination ability towards various

transition metals to effect a desired transformation has distinct advantage to perform reaction in regio, stereo and enantioselective manner. Further, the resulted new methodologies will be applied in targeted molecular synthesis. Hence our research theme will be comprises of appropriate ligand design and their complexation with transition metals with aim towards targeted catalytic reactions. Upon finding the new reactivity, we further will prob into the reaction pathways, isolation of active species and their mechanism.



# Gopakumar Thiruvancheril



## ASSISTANT PROFESSOR

Born in Mannar, Kerala, India, 1978. M. Sc., Mahatma Gandhi University, 2001; Ph.D, Chemnitz University of Technology, Germany, 2006.

National Chemical Laboratory Pune, 2002; Postdoctoral Fellow, Chemnitz University of Technology, 2006-2008; Postdoctoral Fellow, Christian-Albrecht University of Kiel, 2008-2013; Assistant Professor, IIT Kanpur, 2013-.

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## Selected References

Remotely triggered geometrical isomerization of a binuclear complex, *J. Am. Chem. Soc.*, 136, 6163 (2014)

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Influence of Solvophobic Effects on Self-Assembly of Trimesic Acid at the Liquid-Solid Interface, *J. Phys. Chem. C*, 114, 3531 (2010).

HOMO-LUMO Gap Shrinking Reveals Tip-Induced Polarization of Molecules in Ultrathin Layers: Tip-Sample Distance-Dependent Scanning Tunneling Spectroscopy on d8 (Ni, Pd, and Pt) Phthalocyanines, *J. Phys. Chem. C* 112, 2529 (2008).

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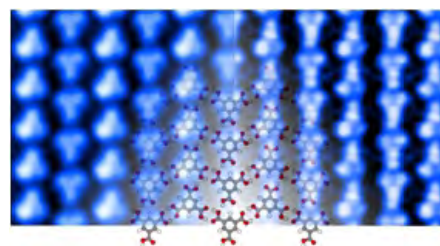
Structure and electronic properties of molecules at interface of metal or semiconductor are of great importance in molecular semiconductor industry. The interest on molecular materials is fuelled due to its small size, highly tunable magnetic and electronic properties and plenty of choice. In addition they offer the unique self-assembling property through which one may design any complex structure, even a most complicated design as in animate systems.

Some molecules imitate electronic functionalities like switches, diodes, rectifiers and wires. These molecules - generally called - functional molecules are candidates for future electronic devices based on single molecules.

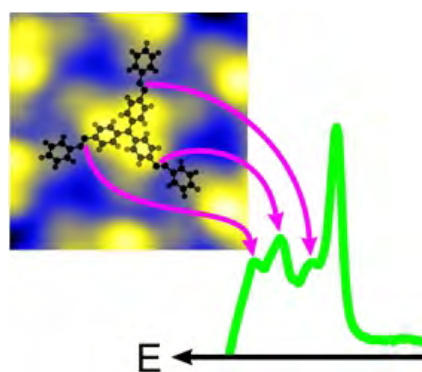
In addition to technological applications the molecules at interface are also of fundamental importance. They do behave different to their bulk counterpart. For example a square planar Fe-porphyrine behave like a square pyramidal structure on Au(111) surface, for which the 5<sup>th</sup> ligand is the surface itself.

We are investigating molecules on surface, especially functional molecules, using Scanning Tunneling Microscope (STM) working at solid-liquid interface at ambient condition. STM working at solid-liquid interface offers a real time investigation of structure, dynamics etc. of molecules at interface. Self assembled monolayer of trimesic (TMA) acid is shown in the figure. TMA is a model system that self-assembles on different surfaces. Its self-assembly may be controlled by the nature of the solvent, concentration etc.

The figure shows a high density structure of TMA (monolayer) controlled by concentration.



A multifunctional molecular switch based on azobenzene on Au(111) surface is shown below. Modification of the molecular symmetry upon adsorption is directly reflected in tunnelling spectrum.



# Yashwant D. Vankar



## PROFESSOR

Born in Varanasi, 1950. M. Sc., Banaras Hindu University, 1971; Ph. D., Banaras Hindu University (Worked at the National Chemical Laboratory, Pune), 1976.

Post-doctoral Fellow, King's College, London, 1976-77; USC Los Angeles, 1977-1979; Rice University, Houston, 1979-1980; Alexander von Humboldt fellow, Universitaet Konstanz, Germany, 1990-91; IIT Kanpur: Lecturer, 1981-1982, Assistant Professor, 1982-91, Professor, 1991-Present, S. K. Roy Memorial Chair Professor, 2006-2009; Mrs. and Mr. J.S. Bindra Memorial Chair Professor, 2013-2016; Fellow, Indian Academy of Sciences, 2002; Fellow, Indian National Science Academy, 2010; Fellow, Royal Society of Chemistry (UK); J. C. Bose National Fellowship of DST.

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## Selected References

N-Halosuccinimide/ $\text{AgNO}_3$ : Efficient reagent systems for one step synthesis of 2-halo glycals from glycals: Application in the synthesis of 2C-branched sugars via Heck coupling reactions. *Org. Lett.*, 16, 1172 (2014).

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Acetyl Chloride-Silver Nitrate Acetonitrile: A Reagent System for the Synthesis of 2-Nitroglycals and 2-Nitro-1-Acetamido Sugars from Glycals, *J. Org. Chem.*, 76, 5832 (2011).

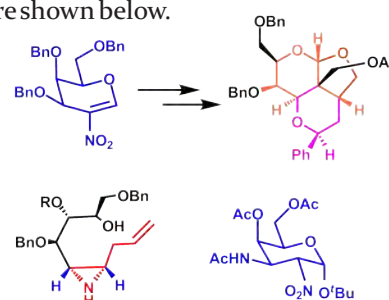
Synthesis of (-)-deoxoprosopphylline, (+)-2-epi-deoxoprosopinine and synthesis of (2R, 3R), (2R, 3S)-3-hydroxypipercolic acids from D-glycals. *J. Org. Chem.*, 75, 4608 (2010).

Synthetic Carbohydrate Chemistry is our main theme of research. More precisely, we are interested in (i) design and synthesis of glycosidase inhibitors (ii) development of newer methodologies to functionalise glycals to obtain highly functionalised carbohydrate synthons (iii) development of newer methods for O-, N- and C-glycosylations. Imino and carbasugars form an important class of compounds with interesting structures and immense biological significance, especially as glycosidase inhibitors, making them as important targets for organic synthesis. Synthesis of naturally occurring monocyclic as well bicyclic iminosugars, and design and synthesis of their analogues is of utmost importance, since glycosidase inhibitors are useful for the treatment of diseases such as diabetes, Gaucher's disease, Fabry's disease, AIDS, etc. Among the monocyclic iminosugars, numerous five, six and seven membered compounds, either naturally occurring or synthetic ones, have been reported in the literature as potent glycosidase inhibitors. Among the bicyclic compounds, indolizidines such as lentiginosine, swainsonine and castanospermine and their analogues are of continued interest, owing to their biological importance and therapeutic value. A few such molecules synthesized by us are shown below.



We are also involved in pursuing the chemistry related to functionalisation of

glycals and also explore the chemistry of C-2 substituted glycals with a view to obtain highly functionalised carbohydrates. Among C-2 substituted glycals, we have explored the chemistry of 2-nitroglycals since they have been recognized as important synthons in carbohydrate chemistry in the recent past. This is because of the presence of a conjugated nitroolefin and an enol ether moiety that offer many possibilities of synthetic manipulations. For example, such a combination makes these substrates useful for the Michael addition, Diels-Alder reactions, (2+3) cycloadditions etc. Besides, the nitro group can be converted to many other useful functionalities such as a carbonyl and an amino group, apart from it being reductively removed. This has led the utilization of 2-nitroglycals as excellent glycosyl donors also. As a consequence, 2-nitroglycals have been utilized in the synthesis of glycoproteins, glycosyl amino acids, and aminosugars via glycosylation as a key step. Besides these, they are used in the synthesis of bicyclic hybrid molecules, fused heterocycles, C-glycosides, 2C-branched sugars etc. Our aim is to develop new methods to procure 2-nitroglycals and also explore new chemistry related to these molecules. Few synthesised molecules are shown below.





# Sandeep Verma



## PROFESSOR

Born in Kanpur, Uttar Pradesh, 1966. M. Sc., Banaras Hindu University, 1989; Ph. D., University of Illinois, Chicago, USA, 1994.

Johns Hopkins Medical Institutions, Baltimore, USA, 1994-1996; Max Planck Institute for Experimental Medicine, Göttingen, Germany, 1996-1997; IIT Kanpur, 1997-; Swarnajayanti Fellow, DST, 2005-2010; Fellow, National Academy of Sciences, India, 2010; Shanti Swarup Bhatnagar Prize, 2010; Fellow, Indian Academy of Sciences, 2011; DAE-SRC Outstanding Investigator Award, 2012; J C Bose National Fellow, DST, 2013; Ranbaxy Research Prize, 2013.

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## Selected References

Purine-stabilized green fluorescent gold nanoclusters for cell nuclei imaging applications, *ACS Appl. Mater. Interfaces* 6, 2185 (2014).

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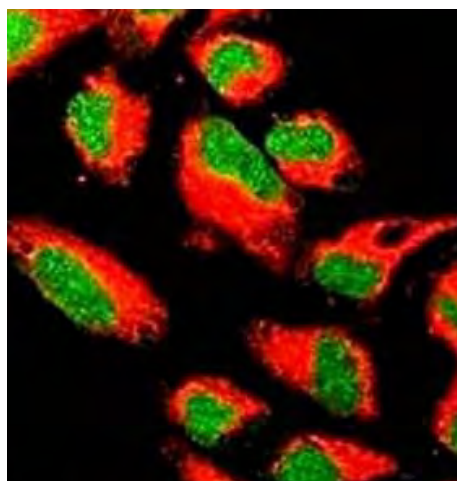
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Characterization of an unprecedented organomercury adduct via Hg(II)-mediated cyclization of N9-propargylguanine, *Chem. Commun.* 47, 1755 (2011).

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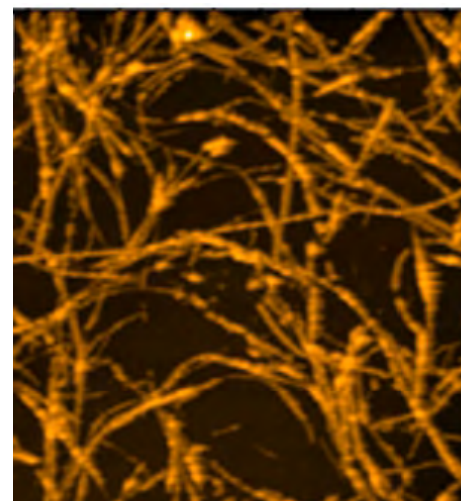
Research program in the Verma group applies bioessential molecules for creating organic frameworks, to study biomimetic processes and to decipher ordered aggregation relevant to certain neurodegenerative diseases. These studies encompass a broad canvass of synthetic organic chemistry, crystallography, microscopy, and cell and material studies.

Our ongoing work on metal-nucleobase interaction focuses on existing knowledge of nucleic acid-metal interactions to craft structurally interesting architectures with outstanding photophysical properties, new materials for gas storage and hybrid electrodes. We have reported formation of entangled networks and extended frameworks, with selective and reversible water vapour and gas adsorption behavior. On another note, a green fluorescent gold nanocluster, stabilized by modified purine ligand, was reported as a stable, nuclear stain for a variety of cancer cells.



Peptide-based self-assembly offers unique entry to construction of soft structures, in order to model molecular mechanisms of aggregation-induced diseases and for designing soft materials with desired properties and functions. It is proposed that precise control over shape and size selectivity in peptide-based nanostructures also offers crucial insight into operating mechanisms associated with protein self-assembly process.

We work on peptide conjugates to address prion protein and Ab aggregation. In this context, we also design small molecules which interfere with protein/peptide aggregation. One such example is inhibition of insulin amyloidogenesis by designed peptide conjugates. Our laboratory is engaged in rational ligand synthesis and inhibition of amyloidogenic diseases.



# Veejendra K. Yadav



## PROFESSOR

Born in Jaunpur, UP, 1956. M. Sc., Banaras Hindu University, Varanasi, 1977; Ph. D., M. S. University, Baroda, 1982.

Postdoctoral Fellow: University of Calgary, Canada, 1983-1984; Memorial University of Newfoundland, St. John's, Canada, 1984-1988; University of Ottawa, Canada, 1988-1989; University of Southern California, Los Angeles, 1989-1990; Visiting Professor: University des Rennes, France, 2002; Tokushima Bunri University, 2002-2003; IIT Kanpur 1990-.

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## Selected References

Route to 2-alkenyl-3-tert-butylidiphenylsilylamines and construction of a tricyclic ring system, *Eur. J. Org. Chem.*, 4163 (2013).

Rearrangement of azetidine into pyrrolidine, *Org. Biol. Chem.*, 10, 4390 (2012).

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Indenes from silylmethyl-substituted cyclopropyl carbinols, *Chem. Commun.*, 2281 (2007).

Total syntheses of (+)-goniopypyrone and (+)-goniofufurones, *Chem. Commun.*, 5232 (2007).

The validity of  $\sigma \rightarrow \sigma^*$ ,  $\sigma \rightarrow \sigma^*$  and  $\sigma \rightarrow \pi^*_{C=O}$  concepts in diastereoselection from NBO analysis, *J. Org. Chem.*, 71, 4178 (2006).

Aziridines and azetidines as masked 1,3- and 1,4-dipoles for formal [3+2] and [4+2] cycloaddition reactions, *J. Am. Chem. Soc.*, 127, 16366 (2005).

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Do the electronic effects of sulfur indeed control the  $\pi$ -selectivity of  $\gamma$ -sulfonyl enones? A reinvestigation, *J. Org. Chem.*, 69, 3866 (2004).

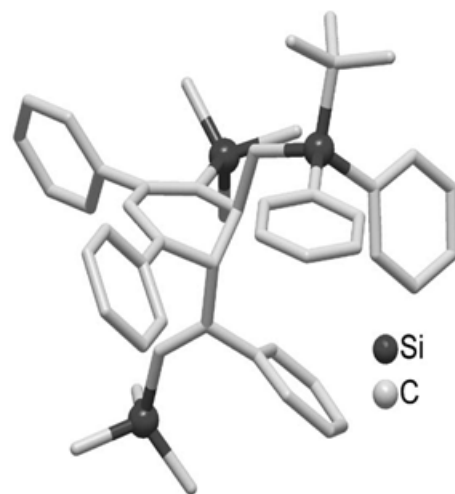
The  $\pi$ -facial selectivity of carbonyl compounds has been at the core of synthetic organic chemistry for long time. The issue has been addressed by many individuals and many theoretical models have been proposed. We have proposed a very simple theoretical model which relies on the geometrical changes around the carbonyl group on coordination with a cation. This model has been successfully applied to many structural scaffolds.

The development of new reactions is another very important area of synthetic organic chemistry research as these allow the assembly of different skeletons with great ease. We have discovered a few new rearrangements and a few new reactions. Prominent among the rearrangements are: (i) 4,5-epoxy-2-oxepanone into 2,6-dioxabicyclo[3.3.0]octan-3-one which has been used by us in the syntheses of (+)-goniofufurone, (+)-7-epigoniofufurone, (+)-goniopypyrone, Hagen's gland lactones and trans-kumausynes, (ii) azetidine into pyrrolidine in a stereospecific manner, and (iii) 3,3-dialkyl-2-silylmethylazetidine into 2-alkenyl-3-silylamines. In regard to the development of new reactions, we have made smart uses of small strained compounds and generated skeletons that are known to possess desirable biological effects.

The protocol developed for the construction of the tetrahydropyran skeleton is free from the often troubling 2-oxonia-Cope rearrangement and it thus provides an easy access to molecules like centrolobine and centrolobinetype. The protocol

generating spiro-indenes from cyclopropyl carbinols may be expanded to develop optical light emitting diodes.

Our group will continue to focus on new reactions development and also the synthesis of molecules of biological interest but using only the home-grown methodologies as the key steps. Issues related to stereoselectivity arising from select structural elements will also be dealt with at theoretical levels.





# Past and Present Heads



Prof. C. N. R. Rao  
1964-66



Prof. M. V. George  
1966-69



Late Prof. P. T. Narasimhan  
1969-72, 1983-86



Late Prof. P. S. Goel  
1972-73, 1986-89



Late Prof. D. Devaprabhakara  
1973-74



Prof. A. Chakravorthy  
1974-77



Prof. S. Ranganathan  
1977-80



Prof. U. C. Agarwala  
1980-83



Prof. S. S. Katiyar  
1989-92



Prof. P. K. Ghosh  
1992-95



Prof. S. K. Dogra  
1995-98



Prof. N. Sathyamurthy  
1998-01



Prof. S. Sarkar  
2002-04



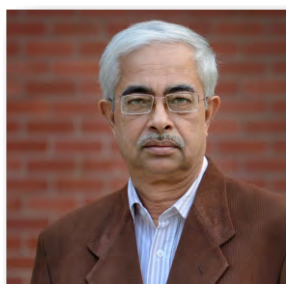
Prof. Y. D. Vankar  
2005-07



Prof. V. Chandrasekhar  
2008-10



Prof. R. N. Mukherjee  
2010-11



Prof. P. K. Bharadwaj  
2012-14



Prof. S. Verma  
2015-





Matrix of  
Faculty Interests

	Synthetic Organic Chemistry	Medicinal Chemistry	Photo Chemistry	Natural Product Synthesis	Bioorganic Chemistry	Organo-metallic Chemistry	Coordination Chemistry	Inorganic Synthesis	Supramolecular Chemistry	Bioinorganic Chemistry	Catalysis	Statistical Mechanics	Theoretical Chemistry	Solid State Chemistry	Material Chemistry	Reaction Dynamics	Spectroscopy and Imaging
Anantharaman, G.						▲	▲	▲	▲						▲		
Angamuthu, R.						▲	▲	▲		▲	▲						
Bera, J. K.						▲	▲	▲	▲		▲						
Bharadwaj, P. K.							▲	▲	▲						▲		
Chandra, A.												▲	▲			▲	
Chandra, M.																	▲
Chandrasekhar, V.						▲	▲	▲							▲		
Dethe, D. H.	▲	▲		▲							▲						
Gadre, S.													▲				
Gajbhiye, N. S.														▲	▲		
Ghorai, M. K.	▲				▲						▲						
Goswami, D.			▲										▲			▲	▲
Keshavamurthy, S.													▲			▲	
Kundu, S. K.						▲		▲	▲		▲						
Moorthy, J. N.	▲		▲						▲		▲				▲		
Mukherjee, R. N.						▲	▲	▲		▲							
Nair, N. N.													▲			▲	
Patra, A. K.							▲	▲		▲							
Prasad, D. L. V. K.													▲	▲	▲		
Ramanathan, G.		▲			▲												
Ramapanicker, R.	▲	▲		▲	▲												
Ranganathan, M.												▲	▲	▲			
Rao, M. L. N.	▲					▲					▲						
Rath, S. P.			▲				▲	▲		▲					▲		
Sadasivam, M													▲				
Sathyamurthy, N.													▲			▲	
Sen, P.																	▲
Singh, A.	▲	▲	▲	▲							▲						
Singh, V. K.	▲			▲							▲						
Sundararaju, B.						▲		▲			▲						
Thiruvancheril, G.														▲	▲		▲
Vankar, Y. D.	▲	▲		▲	▲												
Verma, S.	▲	▲			▲				▲						▲		
Yadav, V. K.	▲			▲									▲				

# Facilities

**T**he *Department of Chemistry* has excellent facilities including a wide range of sophisticated instruments offering technical support to the research activities. Some of the major facilities are listed here.

## Departmental Facilities

### NMR Spectroscopy

The department operates three high field NMR (both 400 and 500 MHz) spectrometers for recording high-resolution spectra from solution-phase samples. NMR spectrometers are run and maintained by dedicated operators who also routinely train and assist students in recording simple 1-D spectra as well as multidimensional hetero-nuclear experiments.

### X-Ray Crystallography

Determination of molecular structures of organic, organometallic and coordination compounds are performed by single crystal X-ray diffraction measurement using two state-of-the-art single crystal X-ray diffractometers (Bruker Apex-II and D8 Quest Single Crystal Microfocus X Ray Diffractometer) equipped with a low temperature device.

### Mass Spectrometry

This facility allows for collection of routine and high-resolution mass spectra under a variety of ionization conditions from the state-of-the-art Waters Q-TOF Premier HAB213 and Waters GCT Premier mass spectrometers.

### Femtosecond Transient Absorption Spectrometer

Early time structural and excited-state dynamics of molecules and materials in the condensed phase can be studied using this facility. The time resolution of the set-up is 120 fs.

### Resonance Raman Spectrometer

A tunable laser source (Argon ion) coupled to a high resolution Raman spectrometer enables us to record resonant Raman spectra of molecules and materials. This technique can be used to probe subtle changes in the structure of a complex molecular system.





## EPR Spectroscopy

Electron Paramagnetic Resonance spectroscopic measurements are done using Bruker EMX300 EPR spectrometer installed in the department. Our facility routinely records EPR spectra of solid, liquid and frozen samples under variable temperature condition.

**Other departmental facilities** include FT-IR spectrometer, UV-vis-NIR spectrophotometer, elemental (CHNSO) analyzer, Mössbauer spectrometer, circular dichroism spectrometer, Picosecond Time-Resolved Fluorimeter, Atomic Force Microscope, powder X-ray diffractometer, Thermo Gravimetric/Differential Thermal Analyser, polarimeter, Parr Hydrogenation apparatus etc. The department has a dedicated computing facility which is separate from the institute facility and is regularly used.



## Institute Facilities

### High Performance Computing Facilities (HPC)

The Institute Computer center hosts a world class high performance computing facility available to all groups on campus. This state-of-the-art 15360 core cluster is based on Intel Xeon E2670 v2X10 2.5 GHz processors with FDR Infiniband network has a peak performance of 300 TF. This facility was ranked 130<sup>th</sup> in the world in November 2013. Several departmental faculties and their students regularly use the HPC cluster and carry out high-end computational research.

### Advanced Centre for Materials Science (ACMS)

Advanced Centre for Materials Science was created with a view to make available major materials preparation and characterization facilities under one-roof. These state-of-the-art research facilities are regularly upgraded, and maintained by suitably trained competent staff. The centre has been serving the needs of the materials community from the institute as well as other academic and industrial

establishments. Several facilities such as Electron microscope, Live Cell Imaging Lab, Mechanical Testing Lab, X-ray photoelectron spectroscopy and Auger spectroscopy facility, Thermal Analysis Lab, X-ray Diffraction Facility, XRF-IRMS Lab are available for the researchers.

### Nanoscience Center

Nanoscience center at the Institute caters the state-of-the-art facility and resources for carrying out research and development activities in the areas of soft nanofabrication. Some of the major equipments at the center are NSOM/Raman/Confocal/AFM, Scanning Electron Microscope with E-beam Lithography, Small Angle and Wide Angle XRD.



# Directions for Visitors

**T**he *IIT Kanpur* campus is located on the Grand Trunk (GT) Road at Kalyanpur, about 16 KM west of Kanpur city.

## Arrival by Air

Visitors can fly to either Kanpur or Lucknow Airport which are well connected with other airports also. Kanpur and Lucknow airports are located about 25 and 90 km, respectively, from IIT campus and will take ~40 mins and two hours to drive by car.

## Arrival by Train

Kanpur Central Railway station is well connected to most cities in North, East and Central India. It is located on the Delhi-Kolkata train route. IIT Kanpur is located at a distance of about 16 kilometers from the Kanpur Central Railway Station. It takes about 40 minutes to drive from Kanpur Central railway station to IIT campus.

## Arrival by Road

Kanpur lies on National Highway 2 (NH2) connecting Amritsar in the North to Kolkata in the East. It passes through New Delhi, Agra, Kanpur, Allahabad and Patna. It is about 480 km from Delhi via this highway. Kanpur is also connected to Lucknow on NH25 and is about 90 km from Lucknow. Kanpur is also connected to Delhi (440 Km) via another highway NH81 passing through Ghaziabad and Aligarh.







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