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P. K. Bharadwaj obtained his Ph.D. from the Indian Institute of Technology Kharagpur in 1979. After spending a year at the Tokyo Institute of Technology as a UNESCO Fellow, he moved to Rutgers University, NJ, USA. At Rutgers, he was first a postdoc and then became Assistant Professor (non-tenure track). In 1985, he moved to University of California, Davis where he worked as a Senior Research Associate before joining IITK in December, 1987. He became a full professor in 1995. His area of research is [Supramolecular Chemistry](#). He has published over 200 research papers including several book chapters.

Macrobicyclic Cryptands Made Livelier : Emission and Other Studies

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Macrobicyclic cryptands have found useful applications in several areas of chemistry, biochemistry and materials research. In these molecules, donor atoms can be placed in strategic positions for having highly stable inclusion complexes with a metal ion. Under suitable conditions utilizing the principles of negative allosteric effect, a metal ion included in the cavity of a cryptand, can be translocated giving rise to interesting properties. Cryptand molecules can be used as excellent skeletons for attachment of different groups that can afford systems again with interesting properties. Some of these aspects of cryptand chemistry will be discussed.

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J. N. Moorthy obtained his masters degree from Bangalore University and worked on solid state photochemistry for his Ph.D from Indian Institute of Science, Bangalore. He pursued postdoctoral research in the laboratories of Profs. J. K. Kochi (Univ. of Houston, Tx, USA), Waldemar Adam (Univ. of Wuerzburg, Germany) and Cornelia Bohne (Univ. of Victoria, BC, Canada) before joining the Department of Chemistry, IIT Kharagpur as a faculty. He moved after a short stint to the Department of Chemistry, IIT Kanpur, where he is currently a full professor.

He has been engaged in a highly diversified and interdisciplinary area of research. His work exemplifies the notion that 'the molecular structure is an embodiment of reactivity and organization'. His three domains of research, viz., organic photochemistry, supramolecular chemistry and mechanistic organic chemistry bear out the importance of structure. With a rational design of molecules, he has demonstrated how reactivity (thermal as well as photochemical) and organization can be manipulated at the molecular level in a pre-determined manner. In a bottom-up approach, he has demonstrated ways, via design and synthesis, to control as well as thwart molecular organization to develop organic functional mimics of inorganic zeolites that are versatile and amorphous organic light-emitting diodes (OLEDs) that exhibit functional utility.

He is a recipient of Alexander von Humboldt postdoctoral research fellowship, Germany (1995-96), Young chemist award, Chemical Research Society of India (CRSI), India (2003), Ramanna research fellowship, Department of Science and Technology (2007-2010), Shanti Swarup Bhatnagar prize in Chemical Sciences (2008) and Bronze medal, CRSI (2010). He is an elected fellow of the Indian academy of Sciences (FASc), Bangalore (2009). He has been a visiting professor at the Univ. of Strasbourg, Strasbourg, France, University of Osaka, Osaka, Japan and Jacobs University, Bremen, Germany.

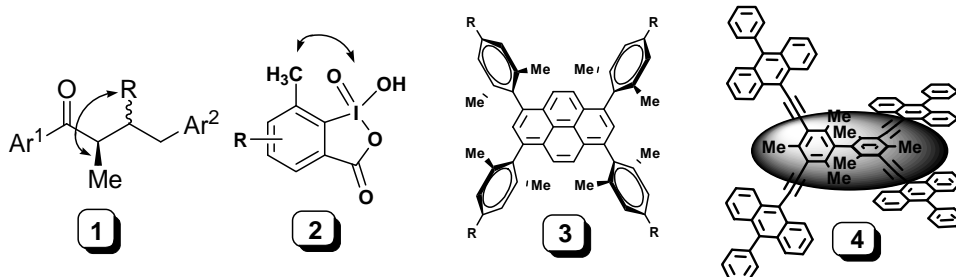
Exploitation of sterics: control of molecular reactivity and organization

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Sterics, originating from the word stereo to mean 3-dimensional perception, has become indispensable in every domain of organic chemistry. We have exploited sterics as an element in the rational design and development of functional organic materials and to control thermal as well as photochemical reactivity. Insofar as the latter is concerned, we have comprehensively established how sterics influence diastereo-differentiating photochemistry of β -alkyl-substituted ketones **1** and thermal oxidation chemistry with IBX derivatives **2**.

Through a rational design of molecular modules, we have developed porous organic materials based on tri- and tetraarylarenes **3** that exhibit kaleidoscopic guest inclusion,³ and organic amorphous materials based on 3-dimensional bimesityl core **4**, which display high glass transition temperatures for application in organic light emitting diodes.⁴



I shall discuss some results of our *de novo* approaches to control reactivity and molecular self-assembly, which is intimately related to material properties.

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Srihari Keshavamurthy is a theoretical chemist in the department of chemistry, IIT Kanpur. Srihari got his PhD degree with William Miller at Berkeley and did a postdoc with Greg Ezra at Cornell. His main interests are in the field of chemical reaction dynamics, mechanisms of intramolecular energy flow and quantum control. He has a long standing interest in the phenomenon of quantum tunneling. The long term program of his group is to establish the unreasonable effectiveness of classical dynamics in reaction dynamics using detailed quantum, classical and semiclassical theories.

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Intramolecular Energy Flow: eigenstates, dynamics and control

Recently, there has been a renaissance of sorts in chemical dynamics with researchers critically examining the validity of the two pillars of reaction rate theory - transition state theory and the Rice-Ramsperger-Kassel-Marcus (RRKM) theory. Interestingly, both the theories have classical dynamics at their foundation and hence significant advances in the field of nonlinear classical dynamics over the last few decades are leading to valuable insights into the intricate dance of molecules.

In this talk I will choose specific examples from our recent research to illustrate the insights that we have gained on the primordial phenomenon of intramolecular vibrational energy flow from a classical-quantum correspondence point of view. More specifically, I will argue that a detailed understanding of both the classical and quantum dynamics of a molecule allows us to assign fairly complicated eigenstates and the potential for formulating ``intelligent'' schemes to control the intramolecular dynamics.



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First Principles molecular dynamics studies on lithium atom solvation in polar binary liquid mixtures

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The preferential ion solvation in mixed solvents is an interesting phenomenon playing important role in solubility and kinetics.^[1,2] I will discuss various structural and dynamical aspects, investigated from first principles molecular dynamics studies, of lithium atom solvation in mixed solvent system like, liquid aqueous-ammonia system at finite temperature. The *ab initio* molecular dynamics simulations have been performed employing the Car-Parrinello molecular dynamics (CPMD) method.^[3,4] This method allows a dynamical propagation scheme within the framework of density functional theory (DFT), where the forces acting on the nuclei are obtained directly from “on the fly” quantum electronic structure calculations.

Spontaneous ionization of lithium atom occurs in the mixed aqueous-ammonia liquid system. The radial distribution functions reveal that Li^+ ion is preferentially solvated by water molecules and the coordination number is mostly four in its first solvation shell. Exchange of water molecules between the first and second solvation shell is very negligible. Li^+ ion and the unbound electron are well separated and screened by polar solvent molecules. Several dynamical features like: diffusion of ion and solvent molecules and orientational relaxations of water and ammonia molecules have been investigated. Hydrogen bond dynamics of solvent molecules have also been investigated in details, and it is found that hydrogen bond lifetimes of water-water, ammonia-ammonia and water-ammonia pairs are different from each other.

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Ashutosh Kumar Mishra has received his Master's degree in chemistry, in 2003, from D. D. U. Gorakhpur University (Gorakhpur, India). In 2005, he received a fellowship from CSIR, India and joined Indian Institute of Technology Kanpur, under the supervision of Prof. Sandeep Verma, as doctoral fellow. His research mainly focuses on designing and synthesis of modified adenine analogues and exploring their interaction with transition metal ions, especially with copper and silver for various purposes ranging from catalytic and DNA cleavage activities, development of fluorescent sensors, generation of aesthetically pleasing supramolecular architectures and their facile deposition on surfaces.

Molecular structure and properties of metal-adenine frameworks

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Modified nucleobases offers versatile platform for metal coordination which could be used as model system mimicking natural analogue to investigate metal binding propensity. These interaction could also be utilized to generate interesting supramolecular architectures having potential applications in the various fields, ranging from catalysis, fluorescent sensor, construction of nucleic acid nanostructures, to name a few.

Our group have been systematically exploring interaction of metal ions with modified adenine nucleobases for various purposes ranging from metallated-polymeric matrix displaying catalytic activity; to the generation metallated complexes exhibiting aesthetically pleasing supramolecular architectures having propensity to form ordered structures onto surface and luminescent behavior.¹ The present report will describe interesting crystallographic aspects of metal complexes of modified adenine analogues leading to the generation of higher order supramolecular architectures; selective sensing of silver ions *via* excimer formation and magnetic properties.²

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