



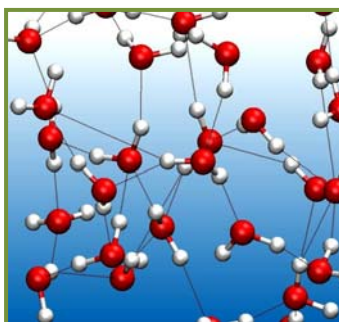
# C. N. R. Rao Lecture

Monday, 6.15 PM, 28<sup>th</sup> February 2011,  
Venue: L-1, Lecture hall complex

Professor Amalendu Chandra,  
Department of Chemistry, IIT Kanpur

## Title: Molecular simulations of liquids and interfaces: An HPC activity at IITK

Abstract: The lecture will deal with our recent studies on chemical dynamics in molecular liquids and interfaces by using a combination of theoretical and computational methods involving first principles simulations, time series analysis, time correlation functions and phenomenological kinetic rate theories. Our primary focus will be on dynamics of vibrational spectral diffusion in hydrogen bonded systems. The correlations of spectral diffusion with simple chemical reactions such as proton transfer processes in aqueous systems will also be discussed.



### About the Donor:

Chintamani Nagesa Ramachandra Rao was born on June 30, 1934 in Bangalore. In 1958, he completed his Ph.D. from Purdue University. In 1958, he became a research chemist at the University of California at Berkeley. Returning to India in 1959, he worked as a lecturer at the Indian Institute of Science in Bangalore. From 1963-76, he was a Professor of Chemistry at the IITK. During 1984-89, he was the Director of the IISc Bangalore.

During his career, Dr. Rao has published more than 25 books and 700 research papers. Concurrent with his academic excellence, he was appointed as Chair of the Scientific Advisory Council to the Indian Prime Minister in 2005. He has won several international prizes and is a foreign member of the US National Academy of Sciences, American Academy of Arts and Sciences and of the Royal Society (London). He has also been given the high honors of Padma Shri and Padma Bhushan by the Indian Government.

The annual C.N.R. Rao Lecture is supported by a donation received from Prof. Rao.

### Previous Speakers:

Year	Name	Title
2010	Gautam Biswas	Understanding Vapor and Air Bubbles
2009	V. Chandrasekhar	Single-Molecule Magnets
2008	Manindra Agrawal	The P<>NP Problem
2007	R.C. Budhani	Low-Dimensional Superconducting and Magnetic Material of Proven Technology Relevance
2006	Kalyanmoy Deb	Evolution Optimization for problem Solving and Knowledge Discovery
2004	Ashutosh Sharma	Of Small Things and other Stories

### About the Speaker

Amalendu Chandra received his Ph.D. from Indian Institute of Science, Bangalore in 1991. He was an Izaak Walton Killam postdoctoral fellow at the University of British Columbia for two years before joining as faculty at IIT Kanpur in 1993.

Prof. Chandra is currently the Rahul and Namita Gautam Chair Professor in the Department of Chemistry and also the Head of the Computer Centre, IIT Kanpur.

He received the Shanti Swarup Bhatnagar Prize from Council of Scientific and Industrial Research, Government of India, in 2007. His research interests include theoretical and computational studies of chemical dynamics in molecular liquids, interfaces and clusters using both classical and quantum methods.

Prof. Chandra is a fellow of Indian Academy of Sciences, Bangalore. He received Ramanna Fellowship of DST, and Alexander-Von Humboldt Fellowship, Germany.

