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.

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