



BOSE COLLOQUIUM

Friday, 3 January 2014

4.00 pm

Fermion

Speaker:

Prof. Amalendu Chandra

Department of Chemistry, Indian Institute of Technology, Kanpur

Title:

Theoretical studies of chemical dynamics in aqueous systems from first principles simulations

Abstract:

The lecture will deal with our recent studies of chemical dynamics in aqueous systems 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 hydrogen bond fluctuations, vibrational spectral diffusion and multidimensional infrared spectroscopy of aqueous systems. The correlations of spectral diffusion and also of simple chemical reactions such as proton transfer processes with hydrogen bond fluctuations in aqueous systems will also be discussed.
