

INSTITUTE COLLOQUIUM

2ND JULY, 2018 | 03:00 PM | BOSON HALL



Speaker
Prof. Amalendu Chandra
N. C. Nigam Chair Professor
Department of Chemistry
Indian Institute of Technology, Kanpur

Title:

Nonlinear Vibrational Spectroscopy of Aqueous Surfaces from Molecular Dynamics Simulations

Abstract:

We will present our recent theoretical studies of nonlinear vibrational spectroscopy of liquid-vapor interfaces of pure water and water-tertiary butyl alcohol (TBA) systems by using a combination of electronic structure calculations and molecular dynamics simulations. Results will be discussed for second order sum frequency generation (SFG) response from aqueous surfaces using OH stretch as the probe vibrational mode. Dynamics of water in the interfacial region will also be discussed and will be correlated with the spectral and structural results.