

The 593<sup>rd</sup>



**MANA & GREEN**

The 57<sup>th</sup>

# The 9<sup>th</sup> Joint Seminar



**Dynamics of aqueous solutions from first principles simulations**

Chair: Dr. Yoshitaka Tateyama (MANA PI)

**Prof. Amalendu Chandra**

(Indian Institute of Technology Kanpur, India)

The lecture will deal with our recent studies of hydrogen bond fluctuations and time dependent infrared spectroscopy of aqueous solutions by using a combination of theoretical and computational methods involving first principles simulations, population correlation functions, time series analysis and time dependent response functions. Our primary focus will be on dynamics of hydrogen bond fluctuations, vibrational spectral diffusion and multidimensional infrared spectroscopy of aqueous systems. The correlations between the spectral diffusion and hydrogen bond fluctuations in aqueous systems will also be discussed. Effects of ionic and molecular solutes on the dynamics will also be discussed. The current theoretical results will also be compared with available experiments on multidimensional infrared spectroscopy of water and aqueous solutions.

**Venue:** Auditorium, 1F, WPI-MANA Bldg., Namiki-site

**Date:** July 18<sup>th</sup>, Tuesday

**Time:** 13:30-14:30