

# *“Frontiers in Science” Seminar*

## **Prof. Pradipta Bandyopadhyay** **Jawaharlal Nehru University, India**

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Title: Modelling Hydration of Small Molecules with Theory and Machine Learning

Date & Time : June 4, 13:15~14:15

Venue : G101 Science Hall (Sugimoto C.)

**Abstract:** Water is a complex liquid with various anomalous properties such as maximum in density, minimum in the heat capacity. Modeling water has been challenging although attempts to understand it started more than hundred years ago. In our endeavor to understand water, we have modelled complex solvation of inert gases in water with a simple statistical mechanical model by describing water as a mixture of hydrogen bonded and non-hydrogen bonded states. We have also developed different chemistry-inspired Machine learning model to predict hydration free energy of drug like molecules.



School of Science /  
Graduate School of Science

Contact : Toshio Asada

Department of Chemistry

E-mail: asada[at]omu.ac.jp