Lecture Series "*Frontiers in Science*"

Prof. Pradipta Bandyopadhyay

Jawaharlal Nehru University, India

Title: Why and how we do computer simulations of proteins: Explanation with examples

Date & Time : June 3, 13:15～14:45

Venue : G310 Meeting Room (Sugimoto C.)

Lecture Contents: Computer simulation of molecular systems is an extremely important area of research complementing experimental research. In this lecture, an introduction to molecular dynamics (MD) simulation will be given from the scratch. Its connection to theoretical chemistry and technical challenges will be discussed. Application of MD simulation for protein molecules will be illustrated with specific examples.

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"*Frontiers in Science*" Seminar

Prof. Pradipta Bandyopadhyay

Jawaharlal Nehru University, India

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.

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