Statistical mechanics of biomolecular solution and its application to in-silico drug design

....

Overview

Statistical mechanics is the theory to describe properties of systems with a large number of degrees of freedom. It is the basis for understanding a molecular system of many particles. A firm foundation in statistical mechanics is necessary to understand the behaviour of macromolecular systems, which is the aim of this course.

This course is organized in two modules that should be taken together. The topics in Module A will expose the participants to the basics of statistical mechanics, such as concept of ensemble, Boltzmann statistics, partition function, and pair correlation function. In Module B, application of statistical mechanics to molecular system will be introduced. The course will discuss how an advance theory like reference interaction site model (RISM) can be used in the context of in-silico drug design.

Computational Lab work will be part of the course. Participants will be given assignments to help them to understand the theory better.

Modules	A: Introduction to statistical mechanics: January 27 - February 2 B: Statistical mechanics and in-silico drug design: February 3- February 9 Number of participants for the course will be limited to fifty.
You Should Attend If…	▪ you are an expert in statistical mechanics but want to know how to use it for biological problems. ▪ you are a student or faculty from an academic institution interested in learning statistical mechanics and its application. ▪ you are working in an industry in the area of structure based drug design
Fees	The participation fees for taking the course is as follows: **Participants from abroad : US $ 500** **Industry/ Private Research Organizations: Rs. 10,000/-** **For Government Research Organizations: Rs. 5000/-** **For JNU students: Free** **For students of recognized institutions: Rs.1000/-** **For faculty of recognized institutions: Rs.2000/-**
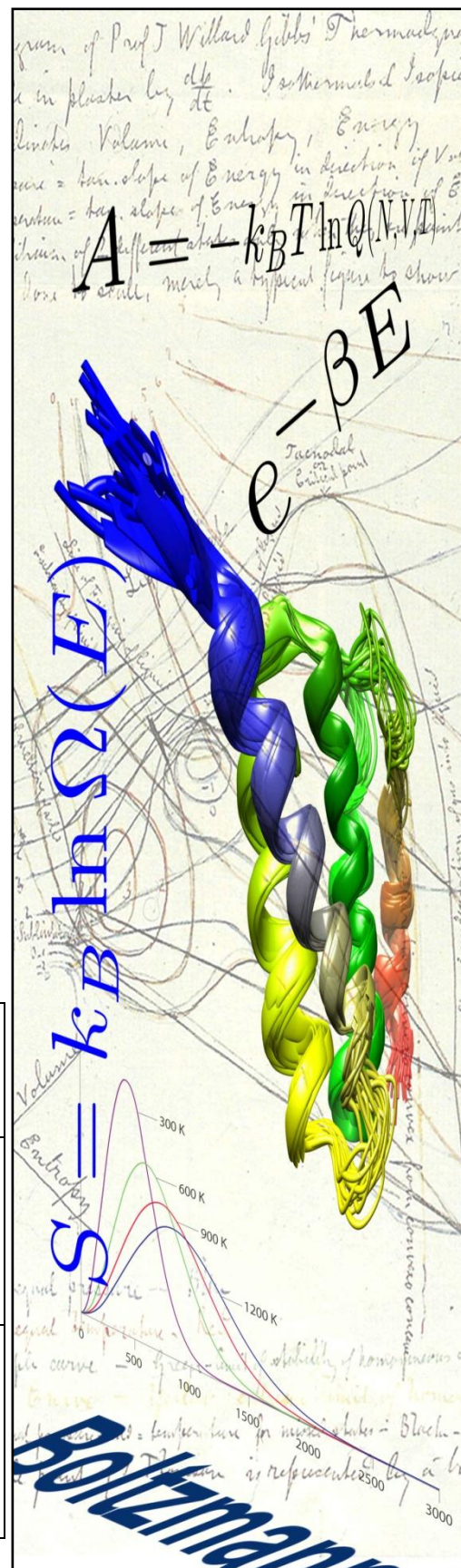
The Faculty

Prof. Fumio Hirata is an emeritus professor at the Institute for molecular science, Okazaki, Japan. He is currently a visiting professor of Ritsumeikan University, Japan. He is considered a pioneer in the area of statistical mechanics applied to chemical and biochemical problems. He is one of the developers of extended reference interaction site model (RISM) method as well as the 3D-RISM theory, which are widely used techniques for understanding a large number of molecular phenomena.

Prof. Pradipta Bandyopadhyay teaches in the School of Computational and Integrative Sciences at Jawaharlal Nehru University (JNU). He is fascinated by statistical mechanics and wants to understand molecular world with it.

Course Co-ordinator

Prof. Pradipta Bandyopadhyay
Phone: 011-26738704
E-mail: praban07@gmail.com

....

http://www.gian.iitkgp.ac.in/