
Seminar

**Driving computer simulation using simple models
and enhanced sampling techniques**

Jagannath Mondal

TCIS, Hyderabad

Understanding physical phenomena at a microscopic level rather than merely reproducing the experimental observables is considered to be one of the major goals for performing computer simulation. Two major bottlenecks hindering the proper usage of computer simulations in this regard are inherent complexity of the experimentally relevant systems and lack of sufficient sampling. In this presentation, I will discuss some of my recent biophysically relevant computer simulations where utilization of simple physics-based models coupled with novel enhanced sampling techniques not only enabled us to gain insight on the underlying physical principle but also set the stage for explaining experimental observation using more atomistically detailed systems. The presentation will mainly cover my recent and ongoing computer simulations on protein-ligand binding and conformational properties of polymers in presence of osmolytes.

Wednesday, Jan 13th 2016

4:00 PM (Tea/Coffee at 3:45 PM)

Seminar Hall, TCIS