School of Nano Science

K.N.Toosi University
Theoretical Physical Chemistry Group

Special Seminar

Enhanced sampling and free energy calculations in molecular simulations

Invited Speaker:
Mehrnoosh Arrar
University of Buenos Aires, Argentina

Abstract:

Atomistic resolution in molecular dynamics simulations limits simulation timescales to the ns- or s regime, often too short for processes of chemical or biological relevance, such as self-assembly or conformational changes in proteins. Accelerated molecular dynamics is a Hamiltonian-modifying technique aimed at enhancing sampling of phase space without losing equilibrium statistical information of the thermodynamic ensemble of interest. Here we will introduce this method and discuss its use in alchemical free energy calculations that would be otherwise difficult to converge.

Thursday, 26 Mordad 1396 (August 17, 2017), 10:00-11:00

Classroom D, Farmanieh Building, IPM