



سمینار هفتگی ماده چگال نرم

Computing Alchemical Free Energy Differences

Najla Hosseini

Institute for Nanoscience and Nanotechnology

Sharif University of Technology

Abstract

On an atomistic scale, free energy calculations are important for our understanding of biological processes, which provides an insight to grasp the various mechanisms. Over the years, many computational methods have been developed to calculate free energy differences such as geometrical (e.g. umbrella sampling) and alchemical methods. In this seminar, I will give an overview of alchemical-free energy methods like thermodynamic integration (TI) and free energy perturbation (FEP). Then, I will compare our simulation studies using TI, FEP, and Hamiltonian replica exchange FEP from the perspective of computational cost.

زمان: شنبه ۱۴۰۰/۰۱/۲۱ ساعت ۱۵:۳۰

مکان: کلاس مجازی آقای دکتر اجتهادی):

<https://vclass.ecourse.sharif.edu/ch/ejtehadi>