سمینار هفتگی ماده چگال نرم

How to parametrize forcefields in coarse-graining approaches

Abstract

In this lecture, I try to introduce some coarse-graining approaches, their applications, and their limitations. Then I try to introduce the parametrization method of the Shape-base Coarse-graining (SBCG) approach. It should be noted that deriving potentials for coarse-grained Molecular Dynamics (MD) simulations are frequently done by solving an inverse problem. Methods like Iterative-Boltzmann-Inversion (IBI) or Inverse Monte Carlo (IMC) have been widely used to solve this problem. The solution obtained by the application of these methods guarantees a match in the radial distribution function (RDF) between the underlying fine-grained system and the derived coarse-grained system. In the SBCG approach, the IBI method is used for parameterization. We are going to look deeper into these methods in the context of the SBCG approach.

Shadi Rahnama

Sharif University of Technology, Nanoscience and Nanotechnology

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