سمینار هفتگی ماده چگال نرم

Deep Potential Molecular Dynamics: A Scalable Model with Quantum Mechanics Accuracy

Abstract

In this talk, a scheme for molecular dynamics simulation with the accuracy of many-body quantum mechanics based on the deep neural network trained with ab-initio data will be introduced. It can be shown that "deep potential molecular dynamics" (DPMD) is an efficient and accurate method for the simulation of many-body potentials and interatomic forces in a variety of systems, from molecules such as chemically bonded species to bulk materials like metallic systems. The neural network model based on this protocol preserves all of the natural symmetries of systems. Additionally, in all of these cases, DPMD can provide results that scale linearly with system size and are essentially indistinguishable from original data. Therefore, this approach can be considered as a very potential procedure in addressing the accuracy-versus-efficiency dilemma in molecular simulations.

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مکان: کلاس مجازی دکتر اجتهادی

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