School of Nano Science

School of PHYSICS

IPM Condensed Matter & Statistical Physics Group

Weekly Seminar

Generating Energy Landscapes of Many-Body Systems using Artificial Neural Networks: Ionic Interactions

Invited speaker: **Dr. Robabe Rasoulkhani**

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Abstract: The accuracy of the results obtained in theoretical simulations critically depends on the reliability of the employed interatomic potentials. While efficient electronic structure methods like density functional theory (DFT) have found a wide application in molecular dynamics simulations of comparably small systems containing up to a few hundred atoms, for an investigation of many interesting problems one has to deal with systems too large for DFT. In recent years artificial neural networks (ANN) have become a promising new tool for the representation of potential-energy surfaces (PES). Due to their flexibility they are able to accurately reproduce a given set of electronic structure data, while the resulting continuous ANN-PES can be evaluated several orders of magnitude faster than the underlying electronic structure calculations. The main drawback of ANN potentials is their intrinsically non-physical functional form. Consequently, large reference data sets from electronic structure calculations have to be available to construct reliable ANN potentials, which are thus more costly to construct than conventional empirical potentials.

In this Seminar, we first present a new physical-based artificial neural networks for ionic crystals so-called CENT. Then, we demonstrate that high-dimensional ANN trained to first-principles data are able to accurately represent the PES of zinc oxide as an ionic material and hence we study the structural properties. Also the applicability of the CENT method to study thermoelectric properties has been investigated for lead chalcogenides. In the first project, some novel structures were discovered and reported. In the second one, machine learning based potential was used to simulate the thermal properties of PbTe and PbS systems. The agreement with ab initio data suggests that this potential could serve as a powerful, fast and accurate tool of investigating the nanostructured thermoelectric materials properties such as morphology of nanostructures.

Wednesday, 7 Azar 1397 (Nov 28, 2018), 14:00-15:00

Seminar Room (classroom A), Farmanieh Building, IPM