数学与系统科学研究院

计算数学所学术报告

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报告题目：

Deep Learning for Multiscale Molecular Modelling

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上午 **9:00-11:00**

报告地点：　科技综合楼三层

311 报告厅

Abstract:

We introduce a series of deep learning based methods for molecular modeling at different scales. We discuss this topic in two aspects: model construction and data generation. In terms of model construction, we introduce the Deep Potential scheme based on a many-body potential and inter-atomic forces generated by a carefully crafted deep neural network trained with ab initio data. We show that the proposed scheme provides an efficient and accurate protocol for a variety of systems, including bulk materials and molecules, and, in particular, for some challenging systems like a high-entropy alloy system. We further show how this scheme is generalized to the context of coarse-graining and free energy computation. In terms of data generation, we present a new active learning approach named Deep Potential Generator (DP-GEN), which is an iterative procedure including exploration, labeling, and training steps. By the example system of Al-Mg alloys, we demonstrate that DP-GEN can generate uniformly accurate potential energy models with a minimum number of labeled data.

欢迎大家参加！