数学与系统科学研究院

计算数学所学术报告

报告人：王涵副研究员

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报告题目：

Deep Potential Molecular dynamics: a scalable model with the accuracy of quantum mechanics

邀请人：　黄记祖博士

报告时间：**2017** 年 **11** 月 **7** 日（周二）

下午 **16:30-18:30**

报告地点：　数学院科技综合楼

三层 **301** 报告厅

报告摘要：

We introduce a new scheme for molecular simulations,

based on a many-body potential and interatomic forces generated by a deep neural network trained with ab initio data. We show that the proposed scheme, which we call Deep Potential Molecular Dynamics (DeePMD), provides an efficient and accurate protocol in a variety of systems, including bulk materials and molecules. In all these cases, DeePMD gives results that are essentially indistinguishable from the original data, at a cost that scales linearly with system size. Moreover, in a few test cases, DeePMD shows good structural transferability to thermodynamic conditions not included in the original training data.

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