数学与系统科学研究院

计算数学所学术报告

报告人：　　陈华杰

（ *北京师范大学* ）

报告题目：

QM/MM methods for crystalline defects with machine-learned interatomic potentials

邀请人：　戴小英 研究员

报告时间：**2021** 年 **9** 月 **10** 日（周五）

上午 **10:00-11:00**

报告地点：数学院南楼

802 教室

Abstract:

We develop and analyze a framework for consistent QM/MM (quantum/classic) hybrid models of crystalline defects, which admits general atomistic interactions including traditional off-the-shell interatomic potentials as well as state of art "machine-learned interatomic potentials". We (i) establish an a priori error estimate for the QM/MM approximations in terms of matching conditions between the MM and QM models, and (ii) demonstrate how to use these matching conditions to construct practical machine learned MM potentials specifically for QM/MM simulations.

欢迎大家参加！