# 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 博士

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报告题目：

**QM/MM Coupling for Crystalline Defect Simulations**

邀请人：　戴小英 副研究员

报告时间：**2015** 年 **8** 月 **26** 日（周三）

上午 **10:00~11:00**

报告地点：　数学院南楼二层

**210** 会议室

# Abstract:

**QM/MM coupling is a widely used technique to perform atomistic simulations of large systems as encountered in materials science and biochemistry. In the context of materials science, the regions of interest such as a defect core, is modeled by an electronic structure model, while the material bulk is modelled with a computationally inexpensive interatomic potential model. We analyze a minimalist electronic structure model: the tight-binding model, and present a new type of locality result. Exploiting this locality, we construct a QM/MM coupling scheme based on energy mixing, where the MM potential can couple well with the QM model. The eciency and accuracy of this construction are shown by rigorous analysis and numerical experiments. This is a join work with Christoph Ortner (University of Warwick), G abor Cs anyi (University of Cambridge) and Noam Bernstein (United States Naval Research Laboratory).**


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