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：

Fermi level in Crystalline Defects with Finite Temperature Tight-Binding

邀请人：　　戴小英 副研究员

报告时间：**2016** 年 **8** 月 **17** 日（周三）

上午 **10:00-11:00**

报告地点：　　数学院南楼七层

702 会议室

Abstract:

We consider a tight binding model for localised crystalline defects with electrons in the canonical ensemble (finite electronic temperature) and nuclei positions relaxed according to the Born–Oppenheimer approximation. We prove that the limit model as the computational domain size grows to infinity is formulated in the grand-canonical ensemble for the electrons. The Fermi-level for the limit model is fixed at a homogeneous crystal level, independent of the defect or electron number in the sequence of finite-domain approximations. We quantify the rates of convergence for the nuclei configuration and for the Fermi-level.This is a joint work with Christoph Ortner (Warwick) and Jianfeng Lu (Duke)

欢迎大家参加！