数学与系统科学研究院

计算数学所学术报告

报告人：**Prof. Lin-Wang Wang**

（ ***Lawrence Berkeley National Laboratory, USA*** ）

报告题目：

Non-adiabatic molecular dynamics simulation to study carrier dynamics

邀请人：　　周爱辉 研究员

报告时间：**2013** 年 **12** 月 **27** 日（周五）

上午 **10:00-11:00**

报告地点：　科技综合楼三层 **311**

计算数学所报告厅

Abstract:

In Non-adiabatic molecular dynamics (NMD), we break away from the Born-Oppenheimer approximation while doing the ab initio molecular dynamics. The electronic configuration does not stay in one adiabatic state. The NMD has been traditionally used to study chemical reactions. Here, we will use NMD to simulate carrier transport in large (>1000 atom) systems. We will discuss the technical issues in such NMD, including the time step one can use, and energy surface hopping algorithms. The talk will be focused on the methodology aspects of the simulation.

欢迎大家参加！