

数学与系统科学研究院  
计算数学所定期学术报告

报告人： 邵嗣烘 副教授

( 北京大学数学科学学院 )

报告题目：

**Time Reversible Born-Oppenheimer  
Molecular Dynamics**

邀请人： 许现民 博士

报告时间：2013 年 12 月 12 日(周四)

下午 16: 00~17: 00

(15: 30~16: 00 茶歇)

报告地点： 科技综合楼三层 311

计算数学所报告厅

## **Abstract:**

**In this talk, we analyze the time reversible Born-Oppenheimer molecular dynamics (TR-BOMD) scheme, which preserves the time reversibility of the Born-Oppenheimer molecular dynamics even with non-convergent self-consistent field iteration. In the linear response regime, we derive the stability condition as well as the accuracy of TRBOMD for computing physical properties such as the phonon frequency obtained from the molecular dynamic simulation. We connect and compare TRBOMD with the Car-Parrinello molecular dynamics in terms of accuracy and stability. We further discuss the accuracy of TRBOMD beyond the linear response regime for non-equilibrium dynamics of nuclei. Our results are demonstrated through numerical experiments using a simplified one dimensional model for Kohn-Sham density functional theory. This is a joint work with Lin Lin and Jianfeng Lu.**

**欢迎大家参加!**