

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**

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报告题目:

**Charge transport calculations: from  
Marcus theory to rt-TDDFT  
simulations**

邀请人: 周爱辉 研究员

报告时间: 2016年6月2日(周四)

下午 16:00-17:00

报告地点: 数学院南楼七层

702 会议室

## **Abstract:**

**In this talk, I will present several recent results in simulating charge transports. Various methods have been used. To study charge transfer between attached molecule and quantum dots, we have used Marcus theory, while to study the nonradiative decay of a defect state, we have calculated all the electron -phonon coupling constants. But to study the mobility of a charge carrier, or the plasmon simulations in an nanoparticle, we have used real-time TDDFT (rt-TDDFT) method. In particular, a new algorithm is developed for the TDDFT method, which allows use to simulate a 50 atom system for 100 fs in a few hours. We have used this approach to study carrier dynamics in nanosystems.**

**欢迎大家参加！**