数学与系统科学研究院

计算数学所学术报告

报告人：　Dr. Jing Shi

　　　　　(Wayne State University)

报告题目：

Quantum transition state theory

邀请人：　陈志明研究员

报告时间：　2009 年 8 月 18 日(周二)

　　　　　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:

Transition state theory is the cornerstone of classical molecular dynamic study of some rare events such as chemical reactions, etc. Quantum effects needs to be taken into account when (but not limited to) light particles and/or low temperature are involved. The high dimensionality of potential energy surface calls for more efficient models without solving Schrodinger equations.

In this talk, I shall discuss various generalizations of classical TST to quantum regime and their applications.

欢迎大家参加！