数学与系统科学研究院

计算数学所学术报告

报告人： **Prof. Qiang Du**

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报告题目：

Computing the transition states of an energy surface

邀请人： 周爱辉研究员

报告时间：**2011 年 10 月 17 日（周一）**

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：

Exploring complex energy landscape is a challenging issue in many applications. Besides locating equilibrium states, it is often also important to identify the transition states given by saddle points. In this talk, we will discuss numerical algorithms such as the dimer methods for the computation of such transition states and present some recently developed mathematical theory. We will consider a number of applications including the study of critical nuclei morphology in solid state transformations. This talk is based on the joint works with Jingyan Zhang, Lei Zhang and Longqing Chen.

欢迎大家参加！