

数学与系统科学研究院

计算数学所学术报告

报告人: **Prof. Zhaojun Bai**

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报告题目:

**Minimization principles of linear
response eigenvalue problems**

邀请人: 周爱辉研究员

报告时间: **2011 年 8 月 29 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:

Linear response eigenvalue problems arise from excitation state calculations of physical systems in the study of collective motion of many particle systems. There are a great deal of recent work and interests in developing efficient simulation techniques for excitation state calculations of molecules for materials design in energy science.

In this talk, we will first present theoretical results on minimization principles of linear response eigenvalue problems and then discuss how to develop conjugate gradient-like algorithms for simultaneously computing the smallest few positive eigenvalues and their associated eigenvectors for excitation state calculations.

This is a joint work with Ren-cang Li, Dario Rocca and Giulia Galli.

欢迎大家参加!