数学与系统科学研究院

计算数学所学术报告

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报告题目：

A Green function method for ab initio electronic structure calculations

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报告时间：2017 年 6 月 22 日（周四）

下午 15:00-16:00

报告地点：　科技综合楼三层

311 报告厅

Abstract:

Ab initio electronic structure calculation based on density functional theory is a very powerful tool for the computational study of physical and chemical properties of materials. A major computational task in the ab initio calculations is to solve the Kohn-Sham equation, which is a Schrodinger equation for one electron moving in an effective potential in local density approximation. In this presentation, I will introduce a Green function approach, in the framework of multiple scattering theory, to the solution of the Kohn-Sham equation, and will discuss a linear scaling method based Green function that allows to meet the computational challenges requiring petascale computing.

欢迎大家参加！