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 framework for adaptive finite element solution of density functional theory

邀请人：　刘歆 副研究员

报告时间：**2016** 年 **7** 月 **26** 日（周二）

上午 **10:00-11:00**

报告地点：　科技综合楼三层

311 报告厅

Abstract：

Density functional theory (DFT) has been playing an important role in a variety of modern sciences such as functional materials design, new energy development, medical imaging. In this talk, we focus on a classical nonlinear phenomenon in the quantum optics, i.e.,high order harmonic generation, and the Kohn-Sham model to introduce the background of density functional theory, and challenges on study from both theoretical and numerical aspects.Then towards resolving the efficiency issue in the simulations, a framework of using adaptive finite element method to solve Kohn-Sham and time dependent Kohn-Sham systems will be introduced in detail. The effectiveness of the framework is shown by several numerical experiments.

欢迎大家参加！