

数学与系统科学研究院

计算数学所学术报告

报告人: 王晓 博士

(中国科学院大学)

报告题目:

**On the Convergence of the
Self-Consistent Field Iteration for
Solving the Kohn-Sham Equation**

邀请人: 刘歆 博士

报告时间: 2013 年 5 月 28 日 (周二)

下午 15:30-16:30

报告地点: 科技综合楼三层 311

计算数学所报告厅

Abstract:

It is well known that the self-consistent field (SCF) iteration for solving the Kohn-Sham (KS) equation often fails to converge, yet there is no clear explanation. In this paper, we investigate the SCF iteration from the perspective of minimizing the corresponding KS total energy functional. By analyzing the second-order Taylor expansion of the KS total energy functional and estimating the relationship between the Hamiltonian and the part of the Hessian which is not used in the SCF iteration, we are able to identify some conditions to ensure global convergence from an arbitrary initial point to and local linear convergence from an initial point sufficiently close to the solution of the KS equation. Our analysis holds under mild assumptions that the second-order derivatives of the exchange correlation functional are uniformly bounded from above.

欢迎大家参加!