FUDAN UNIVERSITY

Applied Math Ph.D. Seminar

Mathematical and Numerical Analysis of Density Functional Theory Models for Metallic Systems

Speaker: Bin Yang (Chinese Academy of Sciences)

Time: 2024-05-23, 16:10 to 17:00

Location: Rm 1801, Guanghua East Tower

Advisor: Aihui Zhou (Chinese Academy of Sciences)

Abstract: In this talk, we investigate the energy minimization model arising in the ensemble Kohn-Sham density functional theory for metallic systems, in which a pseudo-eigenvalue matrix and a general smearing approach are involved. We study the invariance of the energy functional and the existence of the minimizer of the ensemble Kohn-Sham model. We propose an adaptive two-parameter step size strategy and the corresponding preconditioned conjugate gradient methods to solve the energy minimization model. Under some mild but reasonable assumptions, we prove the global convergence for the gradients of the energy functional produced by our algorithms. Numerical experiments show that our algorithms are efficient, especially for large scale metallic systems. In particular, our algorithms produce convergent numerical approximations for some metallic systems, for which the traditional self-consistent field iterations fail to converge. This talk is based on a joint work with Xiaoying Dai, Stefano de Gironcoli, and Aihui Zhou.