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：

Introduction to finite-temperature density functional theory calculations

邀请人：　刘歆副研究员

报告时间：**2017** 年 **11** 月 **9** 日（周四）

上午 **9:30-10:30**

报告地点：数学院科技综合楼

三层 **301** 报告厅

报告摘要：

It is a usual practice to calculate the occupied orbitals for semiconducting, insulating or isolated systems. It differs

significantly in metallic systems and partial occupancies have to be included at the same time. This approach becomes physically significant if the temperature of the system is comparable to characteristic excitation energies. We will derive fundamental formulations of the energy functional and its derivatives with conjugate wavefunctions, partial occupancies, atomic positions, and Lagrange multipliers of the orthonormality constraints. These formulations are built on augmentation charge to accommodate norm-conserving pseudopotentials, ultrasoft pseudopotentials as well as projector augmented wave methods. There are two ways to minimize the finite-temperature density functional with partial occupancies treated as additional variational degrees of freedom: one is direct minimization and the other the self-consistent calculation. We will discuss briefly the direct methods and introduce a consistent update scheme for the partial occupancies. The self-consistent approach split the functional minimization into two subproblems: one is the determination of eigenfunctions and eigenvalues with fixed charge density or potential, the other the self-consistent iteration of charge density or potential. One reason why the

self-consistent schemes are efficient lies probably in the fact that both subproblems can be preconditioned well with plane wave basis. Combining our recent progress, we would like to share our understanding of these two preconditioning.

欢迎大家参加！