数学与系统科学研究院

计算数学所学术报告

报告人：商红慧 副研究员

（ 中国科学院计算技术研究所 ）

报告题目：

Three approaches to solve the coupled perturbed self-consistent field (CPSCF) equation in the density-functional perturbation theory

邀请人：戴小英 研究员

报告时间：**2020** 年 **12** 月 **17** 日（周四）

下午 **14:00-15:00**

报告地点：数学院科技综合楼

311 教室

Abstract:

In this talk, we will show three approaches to get the response density matrix using localized non-orthogonal basis sets. Traditionally, the coupled perturbed self-consistent field~(CPSCF) equation is solved with the sum-over-states method. Here we show that, the CPSCF can be solved with the Sternheimer approach or the purification approach, which only require the occupied states and avoid a sum over unoccupied states. We present a complete derivation of the Sternheimer approach and the purification approach to perturbation theory within the framework of the linear combination of atomic orbital~(LCAO). To demonstrate the capabilities of this method, we have implemented it in the all-electron Fritz Haber Institute ab initio molecular simulations~(FHI-aims) package and applied it to benchmark molecules. For the response properties with respect to the atomic displacement and to the homogeneous electric field, the results are in excellent agreement with the previous traditional method and fully validate the Sternheimer approach and the purification approach.

欢迎大家参加！