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：

Absorption Spectrum Estimation via Linear Response Time-dependent Density Functional Theory

邀请人： 周爱辉 研究员

报告时间：**2015** 年 **8** 月 **17** 日（周一）

下午 **16:00~17:00**

报告地点： 数学院南楼七层

702 会议室

Abstract:

In the time-dependent density functional theory framework, the absorption spectrum of a molecular system can be estimated from the trace of the dynamic polarizability associated with the linear response of the charge density to an external potential perturbation of the ground state Hamiltonian. Although an accurate description of the absorption spectrum requires the diagonalization of the so-called Casida Hamiltonian, there are more efficient ways to obtain a good approximation to the overall profile of the absorption spectrum without computing eigenvalues or eigenvectors. We will describe these methods that only require multipling the Casida Hamiltonian with a number of vectors. They can be used as a fast way to screen molecules and materials. When highly accurate oscillator strength is required for a few selected excitation energy levels, we can use a special iterative method to obtain the eigenvalues and eigenvectors associated with these energy levels efficiently.

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