TDDFT excitation energies, polarizabilities and hyperpolarizabilities of polyacenes and dyes

H. Heinze, A. Görling, N. Rösch

Lehrstuhl für Theoretische Chemie, Technische Universität München, 85747 Garching

A new, non-iterative basis set coupled Kohn-Sham (CKS) method for the efficient calculation of excitation energies, dynamical dipole polarizabilities and hyperpolarizabilities with time dependent density functional theory is presented. The high efficiency of this method rests on the extensive use of auxiliary basis sets. The method is implemented within the framework of our parallel post SCF program RESTDD [1] (RESponse by Time-Dependent Density functional theory). By combining the program RESTDD with the parallel ground state DF program package ParaGauss excitation energies, dynamical dipole polarizabilities and hyperpolarizabilities of large molecules can be treated. Results for polyacens and organical dye molecules are presented and compared to experimental data and accurate ab initio calculations.

[1] A. Görling, H. Heinze, S.P. Ruzankin, M. Staufer and N. Rösch,
J. Chem. Phys. **110**, 2785 1999.