Complex polarization propagator: a theoretical study of molecular properties and spectra.

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In standard response theory, absorption spectra are obtained from residues of so-called response functions and are therefore acquired by solving a generalized eigenvalue problem. In this iterative procedure only the lowest excitations are addressed, therefore the straightforward comparison between standard theory and experiment is impossible in many interesting regions of the spectrum, *e.g.* the X-ray absorption region. This problem can be solved by using the complex polarization propagator approach (CPP)[1], also known as damped (complex) response theory.

A new algorithm for solving complex response equations has recently been developed, namely: the algorithm with symmetrized trial vectors[2]. It is an iterative algorithm based on a subspace approach that combines fast convergence with a very efficient scheme of obtaining new trial vectors, where the coupling between all components are considered explicitly. Calculations of dispersion coefficients[3], one-photon absorption, electronic circular dichroism, magnetic circular dichroism[4] and near carbon K-edge X-ray absorption spectra can be performed at the Hartree-Fock, Kohn-Sham density functional theory and coupled cluster level of theory with the current implementation of the CPP solver in the DALTON program[5]. This has made it possible to perform calculations on nanoparticles[6], which were out of reach of the previous solver.

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