

Abstract Submitted
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Bethe-Salpeter equation without empty electronic states applied to charge-transfer excitations¹ DARIO ROCCA, DEYU LU, Department of Chemistry, University of California, Davis, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California, Davis — We present an approach to compute optical absorption spectra of molecules and nanostructures from first principles, which is suitable for the study of large systems and gives access to spectra within a wide energy range. In this approach, the quantum Liouville equation is solved iteratively within first order perturbation theory, with a Hamiltonian containing a static self-energy operator. This is equivalent to solving the Bethe-Salpeter equation. Explicit calculations of single particle excited states and inversion of dielectric matrices are avoided using techniques based on Density Functional Perturbation Theory [1,2]. In this way, full absorption spectra may be obtained with a computational workload comparable to ground state Hartree-Fock calculations. Applications to the description of charge transfer excitations are presented. [1] D.Rocca, D.Lu and G.Galli (submitted) [2] H. Wilson, F. Gygi and G. Galli, Phys. Rev. B, 78, 113303, 2008; H. Wilson, D. Lu, F. Gygi and G. Galli, Phys. Rev. B, 79, 245106, 2009.

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Dario Rocca
Department of Chemistry, University of California, Davis

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