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Ab initio calculations of optical absorption spectra: Solution of the Bethe-Salpeter equation within density matrix perturbation theory[1]
DARIO ROCCA, UC Davis, DEYU LU, Brookhaven National Laboratory, HUY-VIET NGUYEN, GIULIA GALLI, UC Davis — We present an approach to compute optical absorption spectra 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 [1]. 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]. The calculation and inclusion of GW quasi-particle corrections within this framework are discussed. The efficiency and accuracy of our approach are demonstrated by computing optical spectra of solids, nanostructures and dipeptide molecules exhibiting charge transfer excitations.

[1] D.Rocca, D.Lu and G.Galli, J. Chem. Phys. 133, 164109 (2010).
[2] H. Wilson, F. Gygi and G. Galli, Phys. Rev. B , 78, 113303, (2008).

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