Abstract Submitted
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Calculation of quasi particle energies using a spectral decomposition of the static dielectric matrix: application to molecules and nanoparticles[1] T. ANH PHAM, University of California, Davis, HUY-VIET NGUYEN, University of California, Davis and Center for Computational Physics, Institute of Physics, Vietnam, DARIO ROCCA, GIULIA GALLI, University of California, Davis — We present a novel approach to evaluate quasi particle energies within many body perturbation theory, that substantially improves both the computational efficiency and the numerical accuracy of existing techniques.[2] We use a spectral decomposition of the static dielectric matrix as a basis for the frequency dependent density-density response function, and density functional perturbation theory to avoid the explicit calculation of empty electronic states. A Lanczos-chain algorithm is employed that allows for the evaluation of spectra over a wide frequency range. The numerical accuracy of computed quasi particle energies is controlled by a single parameter. The efficiency and accuracy of our approach are demonstrated by computing vertical ionization potentials and electron affinities of several molecules and diamondoids. Our results are in good agreement with experiment and those reported in the literature using Quantum Monte Carlo calculations.

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T. Anh Pham
University of California, Davis

[2]Huy-Viet Nguyen, T. Anh Pham, D. Rocca and G. Galli, (preprint)

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