

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Application of ab initio many-body perturbation theory with Gaussian basis sets to the singlet and triplet excitations of organic molecules SAMIA HAMED, Chemistry, UC Berkeley, and Molecular Foundry, LBNL, TONATIUH RANGEL, Physics, UC Berkeley, and Molecular Foundry, LBNL, FABIEN BRUNVAL, Materials for Nuclear Energy, French Alternative Energies and Atomic Energy Commission, Paris, France, JEFFREY B. NEATON, Physics, UC Berkeley, and Molecular Foundry, LBNL — Quantitative understanding of charged and neutral excitations of organic molecules is critical in diverse areas of study that include astrophysics and the development of energy technologies that are clean and efficient. The recent use of local basis sets with ab initio many-body perturbation theory in the GW approximation and the Bethe-Salpeter equation approach (BSE), methods traditionally applied to periodic condensed phases with a plane-wave basis, has opened the door to detailed study of such excitations for molecules, as well as accurate numerical benchmarks. Here, through a series of systematic benchmarks with a Gaussian basis, we report on the extent to which the predictive power and utility of this approach depend critically on interdependent underlying approximations and choices for molecules, including the mean-field starting point (eg optimally-tuned range separated hybrids, pure DFT functionals, and untuned hybrids), the GW scheme, and the Tamm Dancoff approximation. We demonstrate the effects of these choices in the context of Thiels' set while drawing analogies to linear-response time-dependent DFT and making comparisons to best theoretical estimates from higher-order wavefunction-based theories.

Samia Hamed
Univ of California - Berkeley

Date submitted: 11 Nov 2016

Electronic form version 1.4