

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Calculating excitation energies with particle-particle and particle-hole random phase approximation using accurate optimized effective potentials YE JIN, YANG YANG, DEGAO PENG, WEITAO YANG, Duke University — With an accurate electron density, one can calculate the optimized effective potential (OEP) which gives Kohn-Sham energies and eigenvectors accurately. Such Kohn-Sham energies and eigenvectors are developed here for applications in excited state calculations. In this work, Kohn-Sham results from OEP with an accurate input electron density, i.e. CCSD density, are used in excitation energy calculations, within the particle-particle and particle-hole random phase approximation (pp-, ph-RPA). Tests on small molecules, for example, BH and CH^+ , matches well with the EOM-CCSD calculation for low energy excited states. For N_2 , CO and H_2O , our method describes the lower excitations well compared with the experimental data and improves the results from pp- and ph-RPA based on approximate density functional approximations. This approach is thus promising for applications in calculating accurate excitation energies.

Ye Jin
Duke University

Date submitted: 06 Nov 2015

Electronic form version 1.4