Efficient determination of excitation energies and absorption spectra of nanoclusters
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Introduction
Theoretical study of nanoclusters is challenging. While the high-level first principle methods are prohibitively expensive for nanoclusters, the semi-empirical methods which could handle them are generally less accurate. The focus of this work is to develop a method to improve semi-empirical models for accurate prediction excitation energies and absorption spectra of nanoclusters. INDO/S Hamiltonian was benchmarked with excitation energies for diatomics from EOM-CCSD. INDO/S model is a drastic approximation to Hartree Fork formalism followed by CIS.

Method
INDO/S Hamiltonian was optimized from a fit to vertical excitation energies from EOM-CCSD/DEF2-TZVPP for Si$_2$, Zn$_2$, Cd$_2$, Cu$_2$, Ag$_2$ and S$_2$ of different inter-atomic separations.

Fit with MAE = 0.17 eV obtained

Results: Transferability of oeINDO

Small clusters : oeINDO, TDDFT and INDO/S compare with MAE 0.25 eV, 0.19 eV and 1.23 eV, respectively.

Large clusters : oeINDO and INDO/S compare with MAE 0.27 eV and 1.16 eV respectively.

References