

# **Benchmarking Ionization Potential and Electron Affinity using DFT/QTP functionals and EOM-CC**

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Density functional theory calculations (DFT) with quantum theory project (QTP) functionals have shown overall improved accuracy to predict properties, such as excitation energies including core, Rydberg, and charge transfer states and fundamental and other excitation gap calculations.

Recently, rigorous evaluation of QTP family (CAM-QTP00, CAM-QTP01, CAM-QTP02 and QTP17) was performed comparing isotropic hyperfine coupling constants calculated from coupled cluster and DFT calculations with widely used functionals and QTP functionals to experiments. It showed the high accuracy of CAM-QTP01 for organic free radical dataset, high accuracy of CAM-QTP01 and CAM-QTP02 for transition metal complex dataset. However, CAM-QTP00 and QTP17 has shown to consistently underperform.

As a continuation of benchmarking of QTP functionals the ionization potential (IP) and electron affinity (EA) obtained from Equation-of-Motion (EOM) Coupled Cluster (CC) and the orbital energies of DFT with QTP functionals are compared. The dataset includes small and large organic molecules as well as transition metal complex molecules. In addition, we compare our results with previous works.