

MULTI-STATE EXTRAPOLATION OF UV/VIS ABSORPTION SPECTRA WITH QM/QM HYBRID METHODS

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In this work, we present a simple approach to obtain absorption spectra from hybrid QM/QM calculations. The goal is to obtain reliable spectra for compounds that are too large to be treated entirely at a high level of theory. The approach is based on the extrapolation of the entire absorption spectrum obtained by individual subcalculations. Our program locates the main spectral features in each subcalculation, e.g. band peaks and shoulders, and fits them to Gaussian functions. Each Gaussian is then extrapolated with a formula similar to that of ONIOM (Our own N-layered Integrated molecular Orbital molecular Mechanics). However, information about individual excitations is not necessary so that difficult state-matching across subcalculations is avoided. This multi-state extrapolation thus requires relatively low implementation effort while affording maximum flexibility in the choice of methods to be combined in the hybrid approach. The test calculations show the efficacy and robustness of this methodology in reproducing the spectrum computed for the entire molecule at a high level of theory.