Describing non-adiabatic interactions with EOM-CCSD theory

Attila Tajti and Péter G. Szalay

Eötvös Loránd University, Institute of Chemistry, Laboratory of Theoretical Chemistry, Budapest, Hungary

The evaluation of the non-adiabatic coupling vector and the interstate vibronic coupling constants within the framework of the EOMEE-CCSD method is presented. Problems arising from the non-Hermitian nature of the theory are discussed in detail. The performance of the new approaches are demonstrated by the comparison of EOMEE-CCSD and MR-CISD results, as well as by the simulation of electronic absorption spectra for small heterocycles within the Linear Vibronic Coupling (LVC) model.