

Equation of motion - double electron attachment

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Equation of motion coupled cluster theory (EOM-CC) provides access to different manifolds of electronic states. Depending on the reference and EOM-CC flavor, one can capture excited states, ionized states, electron attached states, diradicals, and many more. Recent experimental advances like two-photon absorption spectroscopy, laser cooling of molecules have demanded the need for methods that can capture diradicals and doubly excited states. Equation of motion double electron attachment (EOM-DEA) provides accurate, robust, and effective alternatives to target these states. In this study, we successfully implemented the EOM-DEA method and benchmarked the theory. We also implemented the wavefunction analysis module, which can compute different properties like dipole moments, natural orbitals, and natural transition orbitals of the electronic states targeted by this method.