[P6] State-averaged multiconfigurational density-functional theory based on ensembles and range separation

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A hybrid electronic structure method based on the range-separation of two-electron repulsion energy will be presented. While short-range correlation effects are described in DFT for ensembles [1,2,3], this allowing for the simultaneous calculation of both ground and excited states, long-range correlation effects are treated at the SA-DMRG level of -SCF calculation [4]. The new method aims at describing the static correlation using multiconfigurational wave function and, at the same time, the dynamical correlation [5,6,7,8,9]. Results obtained on the prototypical pyramidalized ethylene molecule (which exhibits a conical intersection) [10] will be presented and analyzed.

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