Non-empirical double-hybrid density functionals applied to ground- and excited-state problems

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ABSTRACT

Much progress has been made in developing Double-Hybrid (DH) density functionals, for accurate and robust electronic structure calculations. We will report here non-empirical expressions based on the adiabatic connection model introducing a proper Quadratic Interpolation (QI) function, and the application of these QIDH model for both ground- and excited-state calculations[1]. The systematic benchmarking of these models along the years have proved their accuracy on a wide range of chemical systems and properties of the most interest, benefiting from advances also in the develppment of new exchange-correlation functionals[2]. Additionally, we will address if the lowest-energy singlet and triplet excited-state inversion (Hund's rule violation) in organic molecules can be also predicted correctly with these models[3].

References

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