A simple and accurate non-emperical doubly-hybrid density functional using quadratic approximation of adiabatic connection formula

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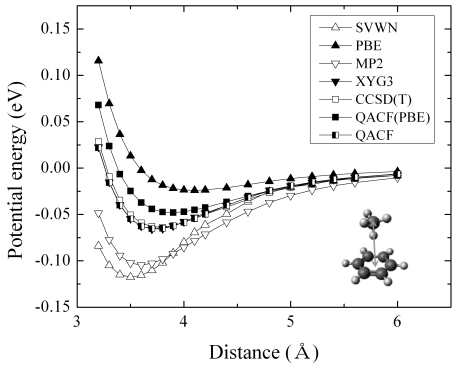
The Kohn-Sham density functional theory(DFT) has been used to predict various properties of molecular system. However most of the density functional, such as LDA, GGA, and hybrid functional, cannot reproduce the heat of formation energy within chemical accuracy of 0.05 eV. Doubly hybrid density functionals (DHDFs) are presently the most accurate density functional due to the inclusion of nonlocality for both exchange and correlation terms, but these functionals are empirically obtained to reproduce experimental data. In this poster, we present an analytic derivation of DHDF based on Becke's adiabatic connection formula. Using quadratic approximation of adiabatic connection formula we obtain a simple analytic expression for a new DHDF whose accuracy reaches 0.1 eV. The test using a methane-benzene complex shows that the new functional also yields an excellent description of the entire potential energy curve that is nearly identical to CCSD(T).



Reference

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