An assessment of XC potentials among hybrid functionals

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ABSTRACT

The exchange-correlation(XC) potential, a crucial component of the Kohn-Sham(KS) equations, is extensively analyzed for 155 hybrid functionals. We utilize the Wu-Yang inverse KS procedure to compute the hybrid XC potentials by inverting electron densities. Full Configuration Interaction(FCI) and CCSD(T) data are utilized as reference. Along with the XC potential, we also analyze the quality of electron density, total energy, and ionization potentials. We find interesting correlations among the quality of exchange-correlation potentials, the long-range Hatree-Fock coefficient, and the vertical ionization potential. We also scrutinize the functionals in terms of functional-driven and density-driven errors. The work underscores the importance of the ability of XC functionals to accurately describe XC potential and its effect on the results of DFT simulations.

References

[1] Kanungo, B.; Zimmerman, PM.; Gavini V.; A Comparison of Exact and Model Exchange–Correlation Potentials for Molecules. *J. Phys. Chem. Lett. 2021, 12,* **2021**, *50*, 12012-12019.

[2] Śmiga, S.; Constantin, LA.; Unveiling the Physics Behind Hybrid Functionals. *J. Phys. Chem. A 124* **2020**, *27*,5606–5614 .