Making the Kohn-Sham Density Functional Theory to Converge to the Right Answer

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The exchange-correlation functionals and potentials in the Kohn-Sham density functional theory are designed empirically. Traditionally, it is difficult to guarantee that they could eventually converge to the right answer like the *ab initio* methods. But the one-particle theory that is designed to converge to the exact answer does exist, such as the correlated orbital theory in which the eigenvalues of all the orbitals equal to the ionization potentials or electron affinities obtained from the equation-of-motion coupled-cluster method. Although the correlated orbital theory is computationally demanding, it is possible to emulate it with the traditional Kohn-Sham density functional theory. Several such types of density functional methods in the QTP family have been designed and evaluated, such as CAM-QTP01 [1], and they could reproduce many ground and excited states more accurately. But some properties computed by these methods still have relatively large errors. During the recent research, these density functional methods are further optimized. This presentation will introduce the principles of the new method as well as the benchmark results.

[1] Jin, Y.; Bartlett, R. J., The QTP family of consistent functionals and potentials in Kohn-Sham density functional theory. *J. Chem. Phys.* **2016,** *145* (3), 034107