Touring from Theoretical Developments through Quantum Simulations guided by Density Functional Theory (DFT)

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Density functional theory (DFT) is often the go-to computational method for solving the electronic structure problems of solids and materials. Although it is an exact theory, one must approximate the exchange-correlation (XC) part, which includes all the many-body interactions. The development of new XC approximations that have insightful physical content and are also accurate and efficient for solids is always desirable. Nevertheless, accurate density functionals approximations are also always the starting point of machine-learning-based functional developments, automated, and high-throughput computational workflow for solids and materials. In my talk, I discuss how present density functional approximations eliminate some of the drawbacks of earlier proposed XC functionals and how one can improve step-by-step the density functional approximations starting from the semilocal DFT to hybrid density functionals to dielectric-dependent hybrids[1–14]. Lastly, I will discuss the future directions of further developments and challenges faced along with new horizons.

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