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Abstract for an Invited Paper for the MAR12 Meeting of the American Physical Society

Progress in fractional perspectives of density functional theory WEITAO YANG, Duke University

Density functional theory of electronic structure is widely and successfully applied in simulations throughout engineering and sciences. However, there are major failures for many predicted properties. These errors can be characterized and understood through the perspective of fractional charges and fractional spins introduced recently. The fractional perspectives offer a possible pathway forward. I will report progress in excited states, spin state splitting, open-shell singlet states, fukui functions and band gaps.