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Local Correction to Reduce Delocalization Errors in Approximate Density Functionals CHEN LI, Department of Chemistry, Duke University, XIAO ZHENG, National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, WEITAO YANG, Department of Chemistry, Duke University — We develop a local correction scheme to reduce delocalization errors in approximate density functionals. A concept of local fractional electron distribution is proposed and corresponding local functions are designed to evaluate its magnitude. Following our previous idea of linearizing each of the nonlinear components in Kohn-Sham density functional, we impose a local linearity condition rather than a global condition. By building our correction functionals in terms of our local functions, we can largely reduce the error in systems that present local fractional electron distribution but no global fractional charge. Our results show that the dissociation curves of diatomic molecules as well as dimer cations can be largely improved. Furthermore, the non-physical ionic product of dissociated molecules by traditional density functionals can be corrected to neutral atoms. We believe the analogous problems in charge transfer systems that are inaccessible for traditional density funcitonals can be correctly handled by our correction functional, and the well-known delocalization error in large extent improved. In addition, our correction scheme maintains the computational efficiency of traditional DFT, enabling it to be applicable to large scale systems.

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