Improving DFT by Quantifying Density Errors

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Density Functional Theory (DFT) is one of the widely used methods for calculating chemical, physical, and electronic properties, and various approximate exchange-correlation (XC) functionals using the Kohn-Sham scheme have been developed and utilized. Clearly, DFT results are highly dependent on the XC approximation. In particular, the approximated XC functional has the self-interaction error unlike the highly accurate values from a high-level calculation such as QMC which requires a large amount of computation even for a small system. Energy errors caused by these functional approximations can be divided and investigated as the functional error and the density-driven error.[1] However, analyzing the two errors individually requires the exact XC functional and density, which is a formidable task. Recently, we devised the density-sensitivity as a practical way to provide an insight into density-driven errors and have shown that it works reasonably well for various calculations.[2] In this presentation, we demonstrate that density-sensitivity can be used to predict the need for density correction in the system of interest and to obtain dramatically improved DFT results using density-corrected DFT in the case of abnormal calculations.[3]

Reference
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