**Correcting DFT problems for the spin-state of transition metal complexes**

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We present calculations for small transition metal complexes using a recently proposed density-corrected density functional theory (DC-DFT) method[1]. Despite its efficiency and reasonable accuracy, density functional theory (DFT) is known to be inaccurate in problematic cases like spin-state changing system. In case of transition metal systems, DFT fails to give accurate spin states consistently and the energy difference between high spin and low spin states are inaccurate. Since controlling spin states in transition metal systems experimentally is extremely difficult, one needs to use computationally costly methods like coupled cluster and quantum Monte Carlo in order to predict preferred spin states. Here we show Hartree-Fock DFT (HF-DFT), one of the simplest ways to perform DC-DFT, gives prediction in spin states with accuracy comparable to coupled cluster results while its computation cost is similar to DFT. In HF-DFT, one evaluates DFT energy on HF densities which results in reducing density-driven error compared to conventional DFT calculation, and has shown promising results in open-shell systems. We believe such improvement in transition metal systems could be expanded to obtain correct spin-densities at no more cost than standard DFT approximations and ultimately to determine magnetization.

1. S. Song, M-C. Kim, E. Sim, A. Benali, O. Heinonen, and K. Burke, J. Chem. Theory Comput. 14, 2304-2311 (2018).