Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Fully self-consistent Fermi-orbital self-interaction correction in density-functional theory[1] ZENGHUI YANG, China Academy of Engineering Physics, MARK PEDERSON, John Hopkins University, JOHN PERDEW, Temple University — Fermi-orbital self-interaction correction(FOSIC) is a new development under the Perdew-Zunger(PZ) SIC framework. It solved the size-extensivity problem of the traditional PZSIC implementation with minimal extra cost associated with the localization of orbitals. The originally published FOSIC algorithm was not self-consistent. This leads to not fully minimized total energy, and can lead to wrong ordering of states in strongly correlated systems. We developed an algorithm for the fully self-consistent FOSIC calculation and implemented it in the NRLmol code. Thanks to the new numerical algorithm, the computational cost increase is minimal going from non-self-consistent to fully self-consistent.

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Date submitted: 13 Nov 2016   Electronic form version 1.4