

Abstract Submitted
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Unitarily Invariant Self-Interaction Corrections to the Uniform Electron Gas MARK PEDERSON, Department of Energy - US, JIANWEI SUN, Department of Physics, Temple University — A new formulation of the self-interaction correction (SIC) to density functional theory (DFT) based upon symmetrically orthogonalized “Fermi-Löwdin orbitals” (FLO) is reviewed [1]. This method leads to an energy that is explicitly unitarily invariant and size extensive and allows for implementation of SIC with the same efficient scaling offered by DFT. Initial applications to small molecules [1] provided orbitals that are similar to past results but yielded SIC-LDA cohesive energies that are competitive with GGA results. Investigations on a uniform electron gas (UEG) provide an additional challenging limit to consider. Results from FLO-based SIC calculations on the UEG, enclosed in a finite box, are presented. In accord with Ref. [2], the FLO-based formulation of SIC finds that localized Wannier orbitals lead to lower energies than plane waves in the exchange-only limit We compare total energies of the uniform electron gas, calculated within DFT, FLO-SIC-DFT, and HF, as a function of functional (including MGGAs[3]), electron number, volume, and Fermi-surface shape.

[1] M.R. Pederson, A. Ruzsinszky & J.P. Perdew, JCP **140**, 121103 (2014).

[2] M.R. Pederson, R.A. Heaton, and J.G. Harrison, PRB **39**, 1581 (1989).

[3] J. Sun, A. Ruzsinszky & J.P. Perdew (this meeting).

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