Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Applications of Fermi-Lowdin-Orbital Self-Interaction Correction Scheme to Organic Systems[1] TUNNA BARUAH, University of Texas at El Paso, DER-YOU KAO, George Washington University, YOH YAMAMOTO, University of Texas at El Paso — Recent progress in treating the self-interaction errors by means of local, Lowdin-orthogonalized Fermi Orbitals offers a promising route to study the effect of self-interaction errors in the electronic structure of molecules. The Fermi orbitals depend on the location of the electronic positions, called as Fermi orbital descriptors. One advantage of using the Fermi orbitals is that the corrected Hamiltonian is unitarily invariant. Minimization of the corrected energies leads to an optimized set of centroid positions. Here we discuss the applications of this method to various systems from constituent atoms to several medium size molecules such as Mg-porphyrin, C_{60}, pentacene etc. The applications to the ionic systems will also be discussed.

[1]De-SC0002168, NSF-DMR 125302

Tunna Baruah
University of Texas at El Paso

Date submitted: 11 Nov 2016 Electronic form version 1.4