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Fermi-orbital Descriptors across the Periodic Table[1] KUSHANTHA WITHANAGE, Physics Department and Science of Advanced Materials Ph.D. Program, Central Michigan University, DER-YOU KAO, Physics Department, Central Michigan University, KOBLAR JACKSON, Physics Department and Science of Advanced Materials Ph.D. Program, Central Michigan University — The optimization of the Fermi-orbital descriptor (FOD) positions is required in the method of Fermi-Lowdin-orbital self-interaction correction (FLO-SIC) in order to minimize the self-interaction-corrected energy.[2] This optimization is carried out using the derivatives of the SIC energy with respect to the FODs. A recent publication[3] showed the optimal FODs for a set of closed shell atoms and that the total energy and ionization energies for these atoms were improved using SIC. Knowing how FODs evolve atom to atom, column to column and row to row over the periodic table is expected be very useful. Clear trends for the atoms may suggest strategies for creating useful starting FOD positions for systems involving many atoms. Such transferability is critical for the efficient application of FLO-SIC to large molecules and clusters. In this talk, we will present a simple unbiased method that we used to find the optimal FODs for atoms up to Z = 36 (Kr). We will present our results and discuss the evolution of and patterns in the FOD positions.

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[2]M. R. Pederson, A. Ruzsinszky, and J. P. Perdew, J. Chem. Phys. **140**, 121103 (2014).
[3]M. R. Pederson, J. Chem. Phys. **142**, 064112 (2015).

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