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High throughput optimization of Fermi-orbital descriptors[1] DERYOU KAO, Physics Department, Central Michigan University, KOBLAR JACKSON, Physics Department and Science of Advanced Materials Ph.D. Program, Central Michigan University — The innovative Fermi-Lowdin-orbital self-interaction correction (FLO-SIC) to density functional theory (DFT) [2] uses N spatial points known as Fermi-orbital descriptors (FODs) to define a unitary transformation between the canonical Kohn-Sham orbitals and the local orbitals used to compute the DFT-SIC total energy. In this talk we describe a simple, unbiased method for optimizing these positions. It involves creating a large number of independent random starting arrangements and then performing a separate local optimization of the FOD positions for each, using derivatives of the total energy with respect to the FOD positions, i.e. FOD forces.[3] A good approximation of the optimal positions can be found by carrying out the local optimization on a frozen space of occupied orbitals. After the approximate positions are found, the occupied orbital space and FODs can be further optimized in tandem to minimize $E^{DFT-SIC}$. Results of using this approach for the Cr atom and Cr_2 will be discussed.

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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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