1159-05-204 **Mark R Pederson***, Mark R Pederson, Department of Physics, El Paso, TX 79968.
Determination of classical representations of quantum phenomena through data-enabled high throughput searchers. Preliminary report.

Fermi-Lowdin orbitals provide a localized representation of quantum wave functions through the use of a quasi classical electronic geometry referred to as Fermi-Orbital descriptors (FODs).[1,2] These orbitals were specifically derived because an improvement of density functional theory, known as the self-interaction correction, required a mechanism for determining unitary matrices that is explicit dependent on and derived from an electronic density that itself is constructed from single-particle wave functions. Determination of the so-called FODs, which define the electronic geometry used for creating these local orbitals ,require a high-throughput search strategy. This strategy will be discussed along with a presentation of the applications of this method to molecules, clusters and qubits.

[1] Fermi orbital derivatives in self-interaction corrected density functional theory. Applications to closed shell atoms, M.R. Pederson, J. Chem. Physics. 142, 0641 (2015).

[1]A multiferroic molecular magnetic quart, A.I. Johnson, F.Islam, C.M. Canali and M.R. Pederson, JCP 151,1741-4 (2019. (Received August 05, 2020)