

# Mean-field Orbital-by-orbital Self-interaction Correction

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## ABSTRACT

We introduce a new method to remove the one-electron self-interaction error in approximate density functional calculations on an orbital-by-orbital basis, as originally proposed by Perdew and Zunger [1]. This method is motivated by a recent proposal by Pederson *et al.* [2] to remove self-interaction that employs orbitals derived from the real-space density matrix, known as FLOSIC (Fermi-Löwdin orbitals self-interaction correction). However, instead of Fermi-Löwdin orbitals, our scheme utilizes columns of the density matrix to determine localized orbitals, like the localization procedure proposed by Fuemmeler *et al.* [3]. In contrast to traditional Perdew-Zunger or FLOSIC, our approach does not add additional optimization parameters and, unlike the average density self-interaction correction of Ciofini *et al.* [4], our method explicitly incorporates localized orbitals, and it can be implemented in a mean-field fashion *via* a multiplicative Hamiltonian. We show details of the self-consistent generalized Kohn-Sham implementation, some illustrative results, and we finally highlight its advantages and limitations.

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## References

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