Abstract Submitted
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Fermi-orbitals for improved electronic structure calculations on biophysically relevant Molecules[1] DER-YOU KAO, Mechanical and Aerospace Engineering , The George Washington University, MARK R. PEDERSON, Department of Chemistry, Johns Hopkins University, JAMES D. LEE, Mechanical and Aerospace Engineering , The George Washington University — An improved density-functional formalism[1,2] proceeds by adopting the Perdew-Zunger expression for a self-interaction-corrected (SIC) density-functional energy but evaluate the total energy based on Fermi Orbitals (FOs). Each localized electron is represented by an FO, determined from the occupied Kohn-Sham orbitals and a semi-classical FO descriptor. The SIC energy is then minimized through the gradients of the energy with respect to these descriptors. Besides providing a review of the calculation of optimization, work here identifies the need for an algorithm which thoroughly searches over initial configurations. The strategy for sampling and prioritizing initial configurations is described. Applications to biophysically relevant spin-polarized molecules, such as Oand molecules containing transition-metal centersare presented. The FO descriptors and FOs for semi-classical and quantum-mechanical understanding of bondingis discussed. Cohesive energies are improved andthe eigenvalues are shifted downward relative to the standard DFT results.Spin-dependent vibrational spectra, as a possible means for spectroscopic determination of the transition-metal moment, are also presented. [1]Pederson et al, JCP 140, 121103(2014). [2]Baruah & Pederson, AAMOPS 64, 153-180(2015).

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