

Abstract Submitted
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Fermi orbital self-interaction corrected electronic structure of molecules beyond local density approximation¹ TORSTEN HAHN, SIMON LIEBING, JENS KORTUS, Institute for Theoretical Physics, TU Freiberg, Germany, MARK PEDERSON, Department of Chemistry, Johns Hopkins University, Baltimore, Maryland 21218, USA — The correction of the self-interaction error that is inherent to all standard density functional theory (DFT) calculations is an object of increasing interest. We present our results on the application of the recently developed Fermi-orbital based approach for the self-interaction correction (FO-SIC) to a set of different molecular systems [1,2]. Our study covers systems ranging from simple diatomic to large organic molecules. Our focus lies on the direct estimation of the ionization potential from orbital eigenvalues and on the ordering of electronic levels in metal-organic molecules. Further, we show that the Fermi orbital positions in structurally similar molecules appear to be transferable. [1] M. R. Pederson, A. Ruzsinszky, and J. P. Perdew, *J. Chem. Phys.* 140, 121103 (2014). [2] M. R. Pederson, *J. Chem. Phys.* 142, 064112 (2015).

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