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Electronic structure of novel charge transfer compounds: application of Fermi orbital self-interaction corrected density functional theory[1] TORSTEN HAHN, Institute for Theoretical Physics, TU Freiberg, 09599 Freiberg, Germany, FLORIAN RCKERL, Institute for Solid State Research, IFW-Dresden, P.O. Box 270116, DE-01171 Dresden, Germany, SIMON LIEBING, Institute for Theoretical Physics, TU Freiberg, 09599 Freiberg, Germany, MARK PEDERSON, Department of Chemistry, Johns Hopkins University, Baltimore, Maryland 21218, USA — We present our experimental and theoretical results on novel Picene/F4TCNQ and Manganese-Phthalocyanine/F4TCNQ donor / acceptor systems. We apply the recently developed Fermi-orbital based approach for self-interaction corrected density functional theory (FO-SIC DFT) to these materials and compare the results to standard DFT calculations and to experimental data obtained by photoemission spectroscopy. We focus our analysis on the description of the magnitude of the ground state charge transfer and on the details of the formed hybrid orbitals. Further, we show that for weakly bound donor / acceptor systems the FO-SIC approach delivers a more realistic description of the electronic structure compared to standard DFT calculations. [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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