

Abstract Submitted  
for the MAR09 Meeting of  
The American Physical Society

**Density Functional Theory of Transition Metal Phthalocyanines**

NOA MAROM, LEEOR KRONIK, Weizmann Institute of Science, Israel — Metal phthalocyanines (MPc's) are a family of highly stable molecules that, as a molecular solid, form organic semiconductors. They have been used in a broad range of applications, e.g., light emitting diodes, solar cells, gas sensors, thin film transistors, and even as single molecule devices. Here, we present a systematic density functional theory (DFT) study of the electronic structure of selected transition metal Pc's: CuPc, NiPc, CoPc, MnPc, and FePc. We critically assess the performance of several semi-local and hybrid exchange-correlation functionals for these systems, and compare the results to experimental photoemission data. For the low-spin systems CuPc, NiPc, and CoPc, we show that semi-local functionals fail qualitatively, primarily because of under-binding of localized orbitals due to self-interaction errors. For the intermediate-spin systems, MnPc and FePc, we show that DFT calculations are extremely sensitive to the choice of functional and basis set with respect to the obtained electronic configuration and to symmetry breaking. However, interestingly, all simulated spectra are in good agreement with experiment despite the differences in the underlying electronic configurations.

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Date submitted: 18 Nov 2008

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