Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

**Describing both Dispersion and Electronic Structure Using Density Functional Theory: The Case of Metal-Phthalocyanine Dimers** NOA MAROM, Weizmann Institute of Science, Israel, ALEXANDRE TKATCHENKO, MATTHIAS SCHEFFLER, Fritz-Haber-Institut, Berlin, LEEOR KRONIK, Weizmann Institute of Science, Israel — Dispersion interactions often determine the structure of crystals and thin layers of organic semiconductors. However, treatment of dispersion is outside the reach of (semi)-local approximations to the exchange-correlation (xc) functional and of hybrid functionals based on semi-local correlation. We offer an approach that treats both dispersion and electronic structure within a computationally tractable scheme, without modifying the xc functional. This is based on adding the leading interatomic dispersion term via pair-wise ion-ion interactions to a suitable non-empirical hybrid functional, with dispersion coefficients and van der Waals radii determined from first-principles using the recently proposed "TS-vdW" scheme. The approach is demonstrated for the case of weakly bound metal-phthalocyanine dimers. It is additionally compared to the semi-empirical M06 functional. We find that both PBEh+vdW and M06 predict the electronic structure and the equilibrium geometry well, but with significant differences in the binding energy and in their different asymptotic behavior.

Noa Marom
Weizmann Institute of Science, Israel

Date submitted: 24 Nov 2009

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