Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Electronic level alignment at a metal-molecule interface from a short-range hybrid functional ARIEL BILLER, Weizmann Institute of Science, Israel, ISAAC TAMBLYN, JEFFERY B. NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory, LEEOR KRONIK, Weizmann Institute of Science, Israel — Hybrid functionals often exhibit a marked improvement over semi-local functionals in the description of the electronic structure of organic materials. Because short-range hybrid functionals, notably the Heyd-Scuseria-Ernzerhof (HSE) functional, can also describe the electronic structure of metals reasonably well, it is interesting to examine to which extent they can correctly describe the electronic structure at metal-organic interfaces. Here, we address this question by comparing HSE calculations with many-body perturbation theory calculations in the GW approximation, or with experimental photoemission data, for two prototypical systems: benzene on graphite and benzene diamine on gold. For both cases, we find that while HSE yields results that are somewhat closer to experiment than those of semi-local functionals, the HSE prediction is still lacking quantitatively by $\sim$1 eV. We show that this quantitative failure arises because HSE does not correctly capture the fundamental gap of the organic, or its renormalization by the metal. These discrepancies are traced back to missing long-range exchange and correlation components, an explanation which applies to any conventional or short-range hybrid functional.

Ariel Biller
Weizmann Institute of Science

Date submitted: 02 Oct 2011

Electronic form version 1.4