Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

First-Principles Studies of Charge Separation in Single-Molecule Heterojunctions[1] PIERRE DARANCET, Molecular Foundry, LBNL, PETER DOAK, Molecular Foundry, LBNL & Department of Chemistry, UC-Berkeley, JEFFREY NEATON, Molecular Foundry, LBNL — Single-molecule heterojunctions, consisting of donor and acceptor moieties linked by covalent bonds and coupled to metal electrodes, provide an interesting model system for understanding processes fundamental to organic solar cells, such as light absorption and charge separation. However, how the covalent contact with metallic leads influence these processes – and metal-molecule interface electronic structure – remains largely unknown. Using density functional theory and many-body perturbation theory, we discuss the influence of the metal contacts and binding groups on junction electronic level alignment for small asymmetric molecules containing covalently-linked moieties based on thiophene, durene and tetrafluoro-, dinitrile-, and metoxy-benzene. Implications for photocurrent and rectification are discussed.

[1]This work was supported by DOE via Helios Solar Energy Research Center. Computational support provided by NERSC.

Pierre Darancet
Molecular Foundry, LBNL

Date submitted: 24 Nov 2009 Electronic form version 1.4