Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Conductance Trends in Single Molecule Junctions Formed Using Donor-Acceptor Links: Theoretical Analysis[1] MAX B. KOENTOPP, LATHA VENKATARAMAN, MICHAEL L. STEIGERWALD, Columbia University, MARK S. HYBERTSEN, Brookhaven National Laboratory — The conductance of single molecule junctions using amine-gold links has been understood based on formation of a donor- acceptor bond involving the N lone pair and the s-orbital on an under-coordinated Au site on the electrode. Experiments probing junctions formed with alkanes terminated by dimethyl phosphines and methyl sulfides also show an unambiguous conductance signature. The structure and bonding in these junctions is analyzed using density functional theory based calculations. Like the amine link, the dimethyl phosphine and methyl sulfide bond to an under-coordinated Au site through a donor-acceptor motif. While the bond energy for the amine and methyl sulfide links are similar (0.6 eV), the dimethyl phosphine is significantly stronger (1.2 eV). Trends in measured junction conductance (amine $<$ sulfide $<$ phosphine) are analyzed in terms of available electronic channels.

[1]This work is supported by the NSF, NYSTAR and the DOE.

Mark Hybertsen
Brookhaven National Laboratory

Date submitted: 30 Nov 2007 Electronic form version 1.4