Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

First-Principles Studies of Single-Molecule Junctions: Conductance and Mechanically-Controlled Switching[1] SU YING QUEK, Molecular Foundry, Lawrence Berkeley National Lab, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University, Seoul, STEVEN G. LOUIE, Department of Physics, University of California, Berkeley and Lawrence Berkeley National Lab, MARK S. HYBERTSEN, Center for Functional Nanomaterials, Brookhaven National Lab, LATHA VENKATARAMAN, Department of Applied Physics and Applied Mathematics and Center for Electron Transport in Nanostructures, Columbia University, J.B. NEATON, Molecular Foundry, Lawrence Berkeley National Lab —
We explore the conductance of amine- and pyridine-Au single-molecule junctions, in the context of recent experiments, with a density-functional theory (DFT)-based scattering state approach. Using a physically motivated self-energy correction, we compute conductance values in good agreement with experiment, in contrast to DFT values that are too large[1]. We investigate quantitatively conductance trends, and demonstrate, together with experiment, that reversible conductance switching can result from mechanically-induced changes in the metal-molecule contact geometry in pyridine-Au junctions. [1] Quek et al, Nano Lett 7, 3477 (2007)

[1]Support: DOE (DE-AC02-05CH11231, DE-AC02-98CH10886), NSF (DMR-0551195, DMR04-39768, CHE-0117752), NYSTAR, NERSC

Su Ying Quek

Date submitted: 21 Nov 2008 Electronic form version 1.4