Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

**First-principles studies of the electronic structure of cyclopentene on Si(100)**[1] SU YING QUEK, Division of Engineering and Applied Sciences, Harvard University, JEFFREY NEATON, The Molecular Foundry, Materials Sciences Division, Lawrence Berkeley National Laboratory, MARK HYBERTSEN, Department of Applied Physics and Center for Transport in Molecular Nanostructures, EFTHIMIOS KAXIRAS, Department of Physics and Division of Engineering and Applied Sciences, Harvard University, STEVEN LOUIE, Department of Physics, University of California, Berkeley & The Molecular Foundry, Materials Sciences Division,Lawrence Berkeley National Laboratory — Small organic molecules on silicon surfaces are promising candidates for active elements in nanoelectronic devices. The interplay between electronic states of the molecule and the silicon surface can change the molecular HOMO-LUMO gap, as well as result in interesting transport properties that depend sensitively on the alignment of molecular frontier orbitals with the silicon band structure. In this work, we determine this alignment quantitatively using the GW method for cyclopentene on Si(100), a prototypical organic-molecule/silicon junction of interest in molecular electronics. We will discuss our results in the context of recent STM experiments that observed negative differential resistance in this system.

[1]This work is supported by NSF(DMR04-39768, CHE-0117752), DOE(DE-AC03-76SF00098), A-STAR & NYSTAR. Computer time was provided by NERSC, NPACI & IHPC.

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Date submitted: 15 Jan 2006 Electronic form version 1.4