Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

**Bipolar molecules with an internal type II heterojunction for nanoscale photovoltaics** GEORGY SAMSONIDZE, MARVIN L. COHEN, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 — Complex organic molecules composed of derivatives of thiophene and naphthalene connected through a bridge show spatially resolved electronic properties corresponding to the HOMO and LUMO states localized on the opposite sides of the molecule, as observed by scanning tunneling spectroscopy. The optical excitation of such molecules is expected to lead to an ultrafast charge separation induced by the intrinsic dipole moment at the donor/acceptor interface, which has potential applications for future nanoscale photovoltaics. We have computed the excited state quasiparticle energies of several bipolar molecules using a first-principles many-electron Green's function approach within the GW approximation for the electron self-energy operator. The renormalizations of the quasiparticle energies induced by the substrate are modeled within an image charge framework. The excitonic properties are calculated by solving the Bethe-Salpeter equation for the electron-hole amplitude. The results of our calculations are compared to available experimental data. This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory's NERSC facility.

Georgy Samsonidze
Dept of Physics, University of California at Berkeley and Materials
Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720

Date submitted: 01 Dec 2009 Electronic form version 1.4