Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Ab-initio calculations of quasiparticle and excitonic properties of low band gap, polythiophene-based polymers[1] FILIPE RIBEIRO, GEORGY SAMSONIDZE, STEVEN LOUIE, MARVIN COHEN, UC Berkeley, and LBL — Electron donor polythiophene-derived polymers coupled with electron acceptor C60 compounds are the basis for the state-of-the-art organic photovoltaic (OPV) technology. However, with an incident photon to converted electron efficiency of only 5%, OPV cells are not yet competitive with conventional inorganic semiconductor technology. One of the limitations is the relatively high energy gap of polythiophene which precludes the absorption of infrared photons. In this work, using the GW approximation and solving the Bethe-Salpeter equation, we compare results of the quasiparticle and excitonic properties of thiophene-, vinylene- and cyanovinylene-based copolymers with lower energy band gaps than polythiophene. The energy band alignments of the polymers and the C60 molecule are also discussed.

[1]National Science Foundation Grant No. DMR07-05941 and the U.S. Department of Energy under Contract No. DE-AC02-05CH11231

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Date submitted: 26 Nov 2007 Electronic form version 1.4