Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Electronic and dielectric properties of organic photovoltaic compounds from first principles ISMAILA DABO, CERMICS, Universite Paris-Est, ANDREA FERRETTI, Istituto Nanoscienze, CNR, CHEOL-HWAN PARK, Department of Materials, Oxford University, NICOLAS POILVERT, Rowland Institute, Harvard University, MATTEO COCOCCIONI, CEMS, University of Minnesota, NICOLA MARZARI, Department of Materials, Oxford University — The initial step towards the design of organic photovoltaic (OPV) devices from first principles is to predict the electronic spectra and dielectric responses of molecular and polymer OPV compounds to quantitative accuracy [*Phys. Rev. B* **71**, 041306 (2005)]. To date, determining the frontier levels and dielectric properties of materials within conventional density-functional theory approximations has been elusive. To address current limitations, orbital-dependent density-functional methods, namely, hybrid density-functional theory (hybrid-DFT) and self-interaction-corrected density-functional theory (SIC-DFT) approximations, represent promising alternatives. In this presentation, we provide a critical comparison of hybrid-DFT and SIC-DFT functionals in determining electronic energies for families of OPV materials. We demonstrate that SIC-DFT based upon Koopmans' condition [*Phys. Rev. B* **82**, 115121 (2010)] is apt at describing donor and acceptor levels within 0.1-0.4 eV and 0.2-0.6 eV relative to experiment. Furthermore, SIC-DFT dielectric responses for semiconducting polymers are predicted in close agreement with more expensive wave-function methods, thereby allowing the accurate and computationally tractable description of donor-acceptor molecular complexes.

Ismaila Dabo
Universite Paris-Est

Date submitted: 02 Nov 2011 Electronic form version 1.4