

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Structural and electronic properties of polymer-silicon semiconductor heterojunctions using hybrid functionals JOSEPH TURNBULL, North Carolina State University, WENCHANG LU, JERRY BERNHOLC, North Carolina State University, Department of Physics, Center for High Performance Simulation; Oak Ridge National Laboratory — Combining organic and inorganic components to form semiconductor heterostructures provides the basis for an enormous number of potential optoelectronic device designs. We report here on the use of hybrid-DFT calculations to study the structural and electronic properties of semiconductor interfaces between silicon and pi-conjugated polymers. Using large supercells and exact-exchange-corrected hybrid functionals, we explore different attachment motifs for polymer monolayers, as well as the role of screening, in particular in the context of predicting semiconductor band-offsets.

Joseph Turnbull
North Carolina State University

Date submitted: 19 Nov 2010

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