Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

**Interaction of Poly(3-hexylthiophene) (P3HT) with NiO (100) Surface: A First-Principles Study**[1] LONGHUA LI, OLEG KONTSEVOI, ARTHUR FREEMAN, Northwestern University — Recent experiments show that NiO outperforms PEDOT:PSS as a hole transport layer in organic photovoltaic (OPV) cells; they also demonstrate that the device performance strongly depends on the composition of the NiO surface, e.g., $O_2$-plasma treated NiO exhibits higher performance than as-deposited NiO. Thus, the polymer/NiO interfacial atomic structure plays a critical role for improving OPVs performance. We model the P3HT/NiO(100) interface by employing DFT calculations to explore the structural and electronic properties and the role of O at the interface. Our results show that in the most energetically favorable interfacial structure the P3HT backbone is aligned along the Ni-O direction. The different roles of the P3HT backbone and side-chain at the interface are presented. Our calculations suggest that side-chains could be used to enhance the interaction of polymer and NiO surface due to a significant contribution to the adsorption energy from the P3HT side-chains. A strong electronic coupling is found between carbon from the P3HT backbone and oxygen of the NiO(100) surface; such C-O coupling may be a possible reason why $O_2$-plasma treatment of NiO results in enhanced device performance.

[1]Supported by the ANSER Center, an EFRC funded by the DOE under Award Number DE-SC0001059

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Date submitted: 13 Nov 2013 Electronic form version 1.4