

Abstract Submitted  
for the MAR07 Meeting of  
The American Physical Society

**Theoretical Insights on Interfacial Charge Transfer across the  
P3HT/Fullerene Photovoltaic Heterojunction from ab Initio Calculations**

YOSUKE KANAI, JEFFREY C. GROSSMAN, Berkeley Nanosciences and Nano-engineering Institute (BNNI), University of California, Berkeley — Within the current effort to develop more efficient and less expensive solar cell devices, the polymer/fullerene photovoltaic (PV) structure is considered to be very promising. The crucial component of such a PV structure is the nano-scale heterojunction interface of the polymer and the fullerene. This interface must facilitate the dissociation of the exciton which is formed in the polymer, so that separated charges can be generated across the interface. Our current understanding of the charge separation mechanism at an atomistic level is rather limited, slowing the progress in the structural design of the heterojunction interface. We employ ab initio calculations to investigate and characterize the charge transfer state which is responsible for the charge separation process. Our results elucidate several important phenomena regarding this mechanism, which lies at the heart of higher power conversion efficiency in polymeric solar cell devices.

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Date submitted: 01 Dec 2006

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