Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Prediction of enhanced photovoltaic performance of amorphous silicon solar cells with filled nanopores JEFFREY GROSSMAN, JOO-HYOUNG LEE, Massachusetts Institute of Technology — We propose a novel hybrid structure for improving the efficiency of thin-film amorphous silicon solar cells. Using *ab initio* calculations, we demonstrate that nanoporous, amorphous silicon (pa-Si), when filled with polythiophene (PT) inside the pores, forms a staggered gap (type II) heterojunction at the interfaces, where both the highest occupied and the lowest unoccupied molecular orbitals of PT are positioned in energy higher than those of pa-Si. Furthermore, we find that while the absorption coefficient (α) of pa-Si is significantly reduced from that of bulk amorphous Si (a-Si), inclusion of PT recovers α to the values of a-Si and even higher at thicknesses of $\sim 1\mu$m. These results suggest that such a hybrid material, which from a manufacturing standpoint may be substantially easier to scale up than nanowire-based approaches, could greatly enhance the hole mobility in the active layer, which is one of the main reasons for poor efficiency in a-Si solar cells.

Joo-Hyoung Lee
Massachusetts Institute of Technology

Date submitted: 19 Nov 2010 Electronic form version 1.4