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Ideal Energy-Level Alignment at the ZnO/P3HT Photovoltaic Interface[1] KEIAN NOORI, FELICIANO GIUSTINO, Department of Materials, University of Oxford — Despite the significant progress made during the past decade, hybrid organic-inorganic photovoltaic devices comprising P3HT and ZnO still suffer from low short-circuit currents and moderate open-circuit voltages. These barriers call for a detailed examination of the atomic-scale physics underlying the energy-level alignment at the ZnO/P3HT interface, which is of critical importance if we are to understand what is the maximum ideal open-circuit voltage for this class of solar cell. Here we present the results of a first-principles study [1] on large model interfaces between ZnO and P3HT. Using a combination of density-functional theory (DFT) and post-DFT methods based on hybrid functionals, we analyze the atomic structure and energetics of the semiconductor/polymer interface, as well as the interfacial energy-level alignment. We explore the effect of charge transfer on the ideal open-circuit voltage and identify a failure in the standard electron affinity rule. We determine a maximum ideal open-circuit voltage of $\sim$2 V, which suggests that there is significant room for enhancing the performance of ZnO/P3HT solar cells by optimizing the interface at the nanoscale.

[1] K. Noori, F. Giustino, Adv. Funct. Mater. DOI:10.1002/adfm.201201478 (2012).

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