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Electronic couplings in organic/ZnO hybrid structures for photovoltaics NA SAI, The University of Texas at Austin, KEVIN LEUNG, Sandia National Laboratories, JAMES R. CHELIKOWSKY, The University of Texas at Austin — Organic-inorganic hybrid structures are promising for photovoltaic applications. Interfacial charge separation and charge transfer must be optimized for efficient power conversion in these systems. While the role of these fundamental processes in interfacial structures has been recognized, the complex interplay between the crystal structure, interfacial molecular orientations, and electronic structure in organic-inorganic interfaces is not well understood at the atomic level. We have carried out large scale first principles calculations of the interfacial energy level alignment and electronic coupling between oligothiophene and ZnO for different molecular orientations at the interface. This allows us to elucidate the geometric dependence of the electronic interactions between the organic molecule and the substrate. The work is supported by EFRC:CST Energy Frontier Research Center funded by the U.S. DOE under Award number DE-SC0001091 and Texas Advanced Computing Center. KL is also supported by the DOE under Contract DE-AC04-94AL85000. Sandia is a multiprogram operated by Sandia Corporation, a Lockheed Martin Company, for the U.S. Deparment of Energy.

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