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Morphology in Hybrid Oxide/Polymer Core-Shell Nanowire Photovoltaics JIE JIANG, SOHRAB ISMAIL-BEIGI, Yale University — We use first principles theory (DFT) to gain insight into the Poly(3-hexylthiophene) (P3HT)-ZnO nanowire binding morphologywhere the P3HT is bound to ZnO via SiO_3 linkers [1]: understanding the experimentally realized morphology is the first step in trying to predict and enhance electronic energy alignments conducive to photovoltaic operation. For large diameter ZnO nanowires, the morphology is that of P3HT bound to the $(10\bar{1}0)$ surface of ZnO. The existence of a lattice mismatch of the ZnO surface and the polymer backbone creates a competition between linker binding and strain energy. We solve this realization of the classic Frenkel-Kontorova model based on ab initio parameters to obtain the lowest energy binding morphology on the surface. For small ZnO nanwire diameters, curvature effects become important: the P3HT polymer must bend around the nanowire, and the reduction of linker spacing due to curvature enlarges the lattice mismatch for helical wrappings. We use DFT to estimate these curvature energies, and we predict a morphology change from helical wrapping to linear alignment with the nanowire axis at a diameter close to 25 nm. [1] S. Zhang, Adv. Mater. (in press, 2011).

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