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The Poly(3-hexylthiophene) / ZnO (10-10) interface: structure and energetics JIE JIANG, SOHRAB ISMAIL-BEIGI, Yale University — The poly(3-hexylthiophene) (P3HT) polymer on ZnO system is of significant interest for hybrid nanoscale solar energy research and applications. Using density functional theory and periodic supercells, we study the P3HT/ZnO interface where sulfur atoms on the P3HT side chains are used to anchor the polymer onto the ZnO (10-10) surface. We discuss the structure and energetics of the binding modes for low and high polymer coverage. We then apply the Frenkel-Kontorova model to study the likely polymer structures in practice (e.g. dislocation formation to release strain energy). We end with a discussion of the band energy alignment across the interface.

Jie Jiang
Yale University

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