

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Theoretical Investigation of Interface Formation and Electronic Structure for Thiophenes on TiO₂ MARILIA CALDAS, Inst. Physics, University of Sao Paulo, Sao Paulo, Brazil, MARCELO ALVES-SANTOS, CNR Nat. Center nanoStructures and bioSystems at Surfaces (S3), Modena, Italy — Atomistic-level understanding of photovoltaic processes for hybrid polymer-oxide structures is a great challenge. The mechanisms of charge transfer across the interface are not known, the electronic characteristics of the two components are very different, and for the polymer depend strongly on the film morphology. The experimental analysis of the interface is difficult, so theoretical simulations can be of great value, but the study carries severe difficulties. We investigated the formation of the interface between thiophene oligomers and the TiO₂(101)-anatase surface, starting from classical molecular dynamics simulations for oligomer deposition, and proceeding to ab initio calculations based on Density Functional Theory (DFT) for electronic properties. We observed the formation of rough thiophene films, with a majority of molecules oriented almost normal to the surface, also molecules lying-down in the first interfacial layer. The DFT study of an infinite thiophene polymer lying-down on the surface, in that same orientation, indicates electronic coupling through a state at the oxide valence-band top, extended through both materials, which favors charge transfer. We acknowledge support from FAPESP and CNPq, Brazil

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Date submitted: 28 Nov 2009

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