

Abstract Submitted
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Energy Alignment at Organic/Oxide and Organic/Metal Interfaces: The Effects of Molecular Overlayer Thickness on the HOMO/LUMO Gap and Interfacial Dipole¹ CHARLES RUGGIERI, SYLVIE RANGAN, SENIA COH, ROBERT BARTYNSKI, Rutgers, The State University of New Jersey — Dye-sensitized solar cells offer the potential for low-cost production with comparable efficiencies to traditional Si-based solar cells. Energy alignment of the dye orbitals with respect to the band edges of the oxide semiconductor substrate is a key parameter in device performance. Using direct and inverse photoemission, XPS, and STM we have investigated the electronic structure and bonding geometry of zinc tetraphenylporphyrin (ZnTPP) molecules adsorbed on a set of four oxide semiconductor and metallic substrates [TiO₂(110), ZnO(11-20), Ag(100) and Au(111)] at monolayer and multilayer coverages. The vacuum levels of the organic/oxide and organic/metal systems were also measured and the interface dipoles determined. The energy level shifts and the width of adsorbate spectral features are qualitatively different for molecules adsorbed on the oxide versus the metal substrates. The HOMO-LUMO energy separation decreases with decreasing molecular overlayer thickness, which is thought to be due to substrate screening properties, but these shifts occur in different ways for the two classes of substrates. Possible origins of this distinct behavior will be discussed.

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