

Abstract Submitted  
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**Electronic structure of N3 DYE molecules on the TiO<sub>2</sub>(110) surface and on anatase nanoparticle films** ERIC BERSCH, Rutgers University, SYLVIE RANGAN, University of Texas at Dallas, JEAN-PATRICK THEISEN, ROBERT A. BARTYNSKI, JUDITH D. SORGE, DUNBAR P. BIRNIE, Rutgers University — We have used direct and inverse photoemission to measure the occupied and unoccupied electronic states, and their alignment with the band edges of the substrate, of N3 dye adsorbed on the rutile TiO<sub>2</sub>(110) surface and on anatase TiO<sub>2</sub> nanoparticle thin films. In dye-sensitized solar cell applications, the HOMO-LUMO gap determines the useful portion of the solar spectrum, and charge transfer of photoexcited electrons to the substrate depends on the alignment of the LUMO to the TiO<sub>2</sub> conduction band edge. Samples were prepared and passivated with a pivalate layer in UHV, then sensitized in air in a solution of N3 dye in acetonitrile. STM measurements show that the pivalic acid forms an ordered overlayer on the TiO<sub>2</sub>(110) surface and that the N3 dye molecules can be imaged after sensitization. Our spectroscopic measurements show that contamination (presumably from water in the ambient) is significantly reduced and that the N3 HOMO occurs at 1.1 eV above the TiO<sub>2</sub> valence band edge, and the LUMO is found 0.3 eV above the conduction band edge. Comparison with experimental and theoretical values from the literature will be discussed.

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