

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Electronic structure of N3 DYE molecules on the ZnO single crystal and epitaxial film surfaces JEAN-PATRICK THEISEN, ERIC BERSCH, SYLVIE RANGAN, YICHENG LU, ROBERT BARTYNSKI — Most dye-sensitized solar cells use TiO₂ nanoparticle films as the electrode, but ZnO offers an interesting alternative. 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 ZnO(0001), ZnO(11-2), epitaxial ZnO a-plane film surfaces, and ZnO nanopillars. As the unoccupied states of ZnO are of *sp*-character and of relatively low cross section, the LUMO of the dye is easily observed. Samples were prepared and passivated with a pivalate layer in UHV, then sensitized in air in a solution of N3 dye in acetonitrile. As opposed to the case of the TiO₂(110) surface, STM measurements indicate that the pivalic acid does. From UPS, the N3 HOMO is found at ~ 0.8 eV above the ZnO valence band edge, and the LUMO is found ~ 1.5 eV above the conduction band edge for the epifilm. Differences in dye adsorption and orbital alignment for these different ZnO surfaces will be discussed.

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Date submitted: 27 Nov 2007

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