Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Energy level alignment of Zn-tetraphenylporphyrins derivatives adsorbed on wide band gap semiconductor oxides SYLVIE RANGAN, SENIA KATALINIC, RYAN THORPE, ROBERT ALLEN BARTYNSKI, JONATHAN ROCHFORD, ELENA GALOPPINI, Rutgers University — Metalloporphyrins play an essential role in photosynthetic mechanisms and therefore are natural candidates for electron transfer mediator in light harvesting devices. The Zn(II) tetraphenylporphyrins (ZnTPP) derivatives have similar electron injection and charge recombination properties as the important standard ruthenium dye N3 for dye sensitized solar cells, and have shown reasonable performances using TiO_2 or ZnO as substrates. This study compares three different ZnTPP derivatives, for which the selective functionalization of the meso-phenyls, allows to control the adsorption geometry as well the molecule/molecule interaction onto a rutile TiO_2(110) and a wurtzite ZnO(11-20) surface. Valence band states have been probed using ultra-violet photoemission spectroscopy, while the conduction band has been obtained from inverse photoemission spectroscopy. Complementary insights on the adsorption geometries have also been obtained using scanning tunnel microscopy. The electronic structure determined experimentally compares well to the calculated density of states, allowing both a simple understanding of the adsorbate electronic properties, and a direct determination of the ZnTPP derivatives frontier orbitals with respect to the substrates band edges.

Sylvie Rangan
Rutgers University

Date submitted: 27 Nov 2009 Electronic form version 1.4