

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Control of exciton delocalization pathways using ZnTPP functionalization ROBERT BARTYNSKI, SYLVIE RANGAN, SENIA COH, JONATHAN ROCHFORD, ELENA GALOPPINI, Rutgers University — Zn(II)-Tetraphenylporphyrin (ZnTPP) derivatives are attractive candidates for photoinduced electron-transfer mediators in dye sensitized solar cells. We have investigated the influence on solar cells efficiency, of the energy alignment and of the molecular adsorption geometry at the ZnTPP/metal-oxides interface. In this work, using x-ray, UV and inverse photoemission spectroscopies in conjunction with density functional theory (DFT) calculations, we have determined the energy alignment of molecular levels with respect to the substrate band edges for several ZnTPP derivatives adsorbed on ZnO(11-20) and TiO₂(110) surfaces. The ZnTPP derivatives were functionalized with COOH anchoring groups, to allow upright or flat adsorption on the surfaces. While the energy alignment is found similar for all of these systems, large differences in devices efficiencies are observed. We have thus explored the adsorption geometry of the same ZnTPPs at the surface of ZnO and TiO₂ using UV-visible absorption and NEXAFS spectroscopies and scanning tunnel microscopy. It is found that for ZnTPPs, upright adsorption opens deleterious exciton delocalization pathways, due to dipole/dipole interactions competing with electron transfer to the substrate. Choosing the adsorption geometry is thus critical for the electronic pathway control.

Sylvie Rangan
Rutgers University

Date submitted: 11 Nov 2011

Electronic form version 1.4