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Spectroscopy of donor-pi-acceptor complexes for solar cells F.J. HIMPSEL, I. ZEGKINOGLOU, P.S. JOHNSON, Physics Department, University of Wisconsin-Madison, C.D. PEMMARAJU, D. PRENDERGAST, The Molecular Foundry, LBNL, M.-E. RAGOUSSI, G. DE LA TORRE, Dept. Quimica Organica, Universidad Autonoma Madrid, D.F. PICKUP, J.E. ORTEGA, Materials Physics Center, University of San Sebastian — A recent improvement in the design of dye sensitized solar cells has been the combination of light absorbing, electron-donating, and electron-withdrawing groups within the same sensitizer molecule. This dye architecture has contributed to increase the energy conversion efficiency, leading to record efficiency values. Here we investigate a zinc(II)-porphyrin-based complex with triphenylamine donor groups and carboxyl linkers for the attachment to an oxide acceptor. The unoccupied orbitals of these three moieties are probed by element-selective X-ray absorption spectroscopy at the N 1s, C 1s, and Zn 2p edges, complemented by time-dependent density functional theory [1,2]. The attachment of electron-donating groups to the porphyrin ring significantly delocalizes the highest occupied molecular orbital (HOMO) of the molecule. This leads to a spatial separation between the HOMO and the lowest unoccupied molecular orbital (LUMO), reducing the recombination rate of photoinduced electrons and holes.

[1] P. L. Cook, et al., J. Chem. Phys. 134, 204707 (2011).
[2] I. Zegkinoglou, et al., J. Phys. Chem. C 117, 13357 (2013).

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