

Abstract Submitted
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Crystal fields of porphyrins and phthalocyanines P.S. JOHNSON, I. BOUKAHIL, F.J. HIMPSEL, Physics Department, University of Wisconsin-Madison, C. KENNEDY, N. JERSETT, P.L. COOK, Natural Sciences Department, University of Wisconsin-Superior, J.M. GARCIA-LASTRA, Physics Department, Technical University of Denmark — Polarization-dependent X-ray absorption spectroscopy at the N 1s and metal 2p edges is combined with density functional and atomic multiplet calculations to determine the crystal field parameters $10Dq$, Ds , and Dt of transition metal (Mn, Fe, Co, Ni) phthalocyanines and octaethylporphyrins [1]. Octaethyl porphyrins are observed to lie flat on Si with native oxide, while phthalocyanines lie on edge. Strong polarization dependence is found at all edges, which facilitates a unique determination of the crystal field parameters. Crystal field values from PBE density functional calculations provide helpful starting values, which are refined by fitting atomic multiplet calculations to the data. Since the crystal field affects electron-hole separation in solar cells, the systematic set of crystal field parameters obtained here can be useful for optimizing dyes for solar cells.

[1] P. S. Johnson, et al., J. Chem. Phys., to be submitted. See also: P. L. Cook, et al., J. Chem. Phys. 131, 194701 (2009); D. F. Pickup, et al., J. Phys. Chem. C. 117, 4410 (2013).

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