EXAMINATION OF TETHERED PORPHYRIN, CHLORIN, AND BACTERIOCHLORIN SENSITIZERS IN METAL-OXIDE SOLAR CELLS

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Abstract

The performance characteristics of tethered porphyrin, chlorin, and bacteriochlorin sensitizers in regenerative solar cells were evaluated. Incident photon-to-current efficiency was measured for solar cells containing one or more sensitizer and TiO_2 electrodes with different morphologies. To elucidate the molecular origins of the effects of tether and tetrapyrrole macrocycle characteristics on photocurrent production, the measured redox potentials and optical absorption spectra were analyzed in terms of the characteristics (energies, electron-density distributions) of the frontier molecular orbitals obtained from density functional theory calculations. Additionally, first-principle simulations were performed for the production of photocurrent by hypothetical planar and actual films. Collectively, the findings give fundamental insights into the factors that govern the observed differences in photocurrent production characteristics for the different tetrapyrrole sensitizers. In addition, the results provide a framework for further tuning of the properties of these sensitizers to enhance solar-cell performance.