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Chlorophyll-like compounds for dye-sensitized solar cells

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Dye-sensitized solar cells (DSSCs) are a promising alternative for silicon-based solar cells due to their low cost and ease of production [1]. The sensitizing dye is a key component for converting solar radiation into electricity. For high power conversion efficiency (PCE), the dye should absorb strongly in the red to near-infrared region and show a panchromatic response [2]. Donor-π-acceptor (D-π-A) type dyes have shown to produce high PCE, the highest reported being 13% [3]. Porphyrins are an attractive candidate for the π moiety due to their highly versatile structure, tunable π based spectroscopic and electrochemical properties, and excellent stabilities [4].

Chlorophyll exhibits an intense and red absorption band which is ideal for DSSC, but it is unstable. Computational analyses were performed on a series of fictive chlorophyll-based compounds to determine the structural changes that gave rise to the intense and red absorption property. Absorption, magnetic circular dichroism (MCD), and emission spectral data were obtained for chlorophyll and a range of synthetic chlorins and computational studies were carried out to provide further insight on their electronic structure. Coupling calculations to spectral data provided a way of predicting the structural elements that result in the chlorophyll-like electronic state.

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