

## Predicting Larger Absorption Cross-section in Porphyrin Dyes using DFT Calculations

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### ABSTRACT

Porphyrin macrocycles play an important role in designing of fluorophores with superior light harvesting properties similar to that of antennas in biological systems. In this paper, new Zn(II)porphyrin dyes were investigated to improve the performance of the YD2-o-C8 using density functional theory (DFT) and time-dependent density functional theory (TD-DFT) calculations. Effects of various substituted and anchoring groups on basic porphine and Zn(II)porphyrin derivatives were systematically studied at the B3LYP/LanL2DZ level. The absorption spectra of Zn(II)porphyrin derivatives bearing one, two and four anchoring groups in the *meso*-positions were also studied. The calculations showed that a molecule [5, 10, 15, 20-(4-carboxyphenylethynyl)porphyrinato]Zn(II) have large absorption cross-section than available in the existing porphyrin dyes. The results of these calculations would open up enormous possibilities to develop porphyrin dyes characterized by high absorption cross-section for various light harvesting applications.

**KEYWORDS:** Zn(II)porphyrin dyes; DSSCs; DFT; TD-DFT; electronic properties; absorption cross-section

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