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Highly-efficient sensitizer with zinc porphyrin as building block: Insights from DFT calculations

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ABSTRACT

To further improve the photoelectronic conversion efficiency of dye-sensitized solar cell, a series of novel D-π-A dyes with Zn porphyrin as building block are evaluated with theoretical calculations. The effect of relative position of Zn-porphyrin (ZP) on the overall performance of D-π-A dye has been investigated by means of density functional theory (DFT) and time-dependent DFT (TD-DFT) approaches. Through the analyzing the molecular geometry, electronic structure, transport properties and light harvesting and utilization of monomer dyes, dye-III is confirmed to be the most suitable one for DSSC application, due to its smaller HOMO-LUMO energy gap, broader absorption coverage, better transport capability, and larger short-circuit current density. Quantum dynamics simulation illustrates novel dyes constructed in current contribution are faster in electron transfer at dye@TiO_2 interface. The overall efficiency of DSSC could be boosted if ZP unit was incorporated close to the acceptor group in D-π-A dye. Our work is expected to provide theoretical guideline for further designing and screening prospective sensitizers for DSSC.

1. Introduction

Due to its light weight, pollution-free, low cost and easy-processing, with colorful and transparent features, dye-sensitized solar cell (DSSC) as a next-generation photovoltaic device arouse wide attention since the breakthrough work reported by O'regan and Gräzel (1991). In recent years, plenty attempts have been devoted to seeking DSSC device with high performance, which is greatly dominated by the nature of the sensitizer and its complicated interaction with TiO_2 semiconductor. A conceivable strategy to regulate device performance is by means of reasonable molecular engineering on sensitizers.

Photosensitizers, such as metal-free organic dyes, ruthenium complexes, and Zn-porphyrin sensitizers have achieved great success (Xie et al., 2015; Wang et al., 2014; Song et al., 2018a). The high performance of DSSC device can be greatly improved with organic sensitizers by suitable modification on donor (Qian et al., 2016; Zhao et al., 2015; Guo et al., 2012; Raheem et al., 2018), π-spacer (Li et al., 2016; Wen et al., 2016; Zhang et al., 2012, 2016; Namuangruk et al., 2012; Ezhumalai et al., 2017; Irfan et al., 2014; Bourass et al., 2016; Eom et al., 2017; Xia et al., 2015), and acceptor (Wang et al., 2011; Liu and Troisi, 2013; Ganesan et al., 2015; Kenji et al., 2015) subunits. Up to now, organic dyes have made significant progress in DSSC field (Yao et al., 2015a,b,c; Nagarajan et al., 2017; Malzner et al., 2017; Zhang et al., 2017). Except for that, Zn-porphyrin sensitizers have shown an excellent potential due to their stable structure, intense Soret and Q-bands and tunable spectral properties. At present, the cobalt redox-based DSSC has reached a conversion efficiency exceeding 12% (12.3% with YD2-o-C8 dye (Yella et al., 2011) and 13% with SM315 dye (Mathew et al., 2014)). These milestones boost the investigations of organic and Zn-porphyrin sensitizers for developing high efficiency DSSC (Tang et al., 2015; Yang et al., 2017; Wei et al., 2015).

However, in consideration of the limitation brought by individual sensitizer, the co-sensitization of two or more dyes sensitized on the semiconductor films together is regarded as an effective approach to broaden the absorption coverage and enhance the device performance. Apart from that, some of investigations are devoted to designing and synthesizing a new type of sensitizer that incorporates metal-based dyes into D-π-A organic dyes to further improve the solar-to-electricity conversion efficiency.

DSSC with 13% efficiency is achieved through the molecular engineering of porphyrin sensitizers in Mathew et al. (2014). Recently, much of the work reported by Song et al. (2018c,b) and Li et al. (2018)

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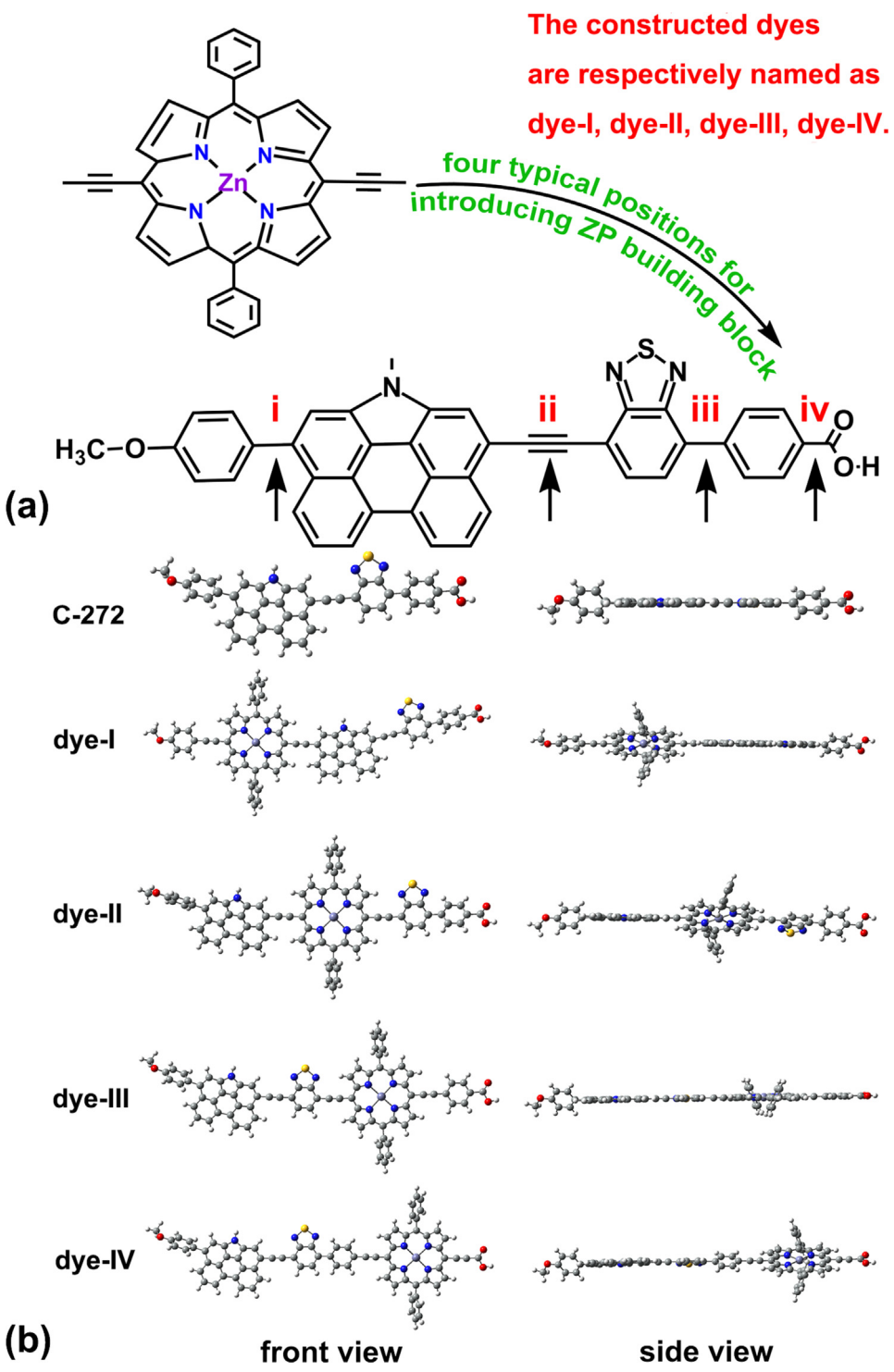

Fig. 1. (a). Schematic structures of the investigated dyes; (b). Optimized ground state structures of the investigated dyes (front view and side view).

has investigated a series of D-π-A Zn-porphyrin dyes in detail, and provided many optimal strategies to further improving the efficiency of DSSC. Kang et al. (2013) investigated the D-π-A structured Zn-porphyrin dyes with bulky fluorenyl substituted electron donor moieties, reporting that this type sensitizers can improve the efficiency significantly due to the combination of merits between organic dye and Zn-porphyrin dye. Pelleja et al. (2014) confirmed that the decoration of porphyrin sensitizers with donor-(π-spacer)-acceptor (D-π-A) structure in which the porphyrin ring core constitutes the π-spacer has led to efficiencies which rival the best Ru(II) polypyridyl dyes (Wang et al., 2012, 2014; Bessho et al., 2010). Our previous work (He et al., 2017a) has suggested that extra donor group and multi-branches could induce remarkable effect on the D-π-A dye. Although all the above investigations focus on designing and synthesising highly efficient sensitizers, how to improve the overall efficiency of D-π-A structured Zn-porphyrin dye from the aspect of molecular engineering are still unknown.

In current contribution, therefore, with the C-272 dye (Yao et al., 2015d) as prototype, we respectively arrange ZP building block onto the four possible positions in C-272 dye to construct novel D-π-A dyes. Yan et al. (2015) have suggested that inserting triple-bond between two