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Computational Studies of the Reactivity Descriptors and the Optoelectronic Properties on the Efficiency Free-Base- and Zn-Porphyrin-Sensitized Solar Cells

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Abstract : This work reports density functional theory calculations of the optimized geometries, molecular reactivity, energy gap,and thermodynamic properties of the free base (H2P) and their Zn (II) metallated (ZnP), bearing one, two, or three carboxylic acid groups using the hybrid functional B3LYP, Cam-B3lYP, wb97xd with 6-31G(d,p) basis sets. When donating groups are attached to the molecular dye, the bond lengths are slightly decreased, which is important for the easy transfer of an electron from donating to the accepting group. For all dyes, the highest occupied molecular orbital/lowest occupied molecular orbital analysis results in positive outcomes upon electron injection to the semiconductor and subsequent dye regeneration by the electrolyte. The ionization potential increases with increasing conjugation; therefore, the compound dye attached to one carboxylic acid group has the highest ionization potential. The results show higher efficiencies of those sensitized with ZnP. These results have been explained, taking into account the electronic character of the metal ion, which acts as a mediator in the injection step, and, on the other hand, considering the number of anchoring groups to which it binds to the surface of TiO2.

Keywords : DSSC, porphyrin, TD-DFT, electronic properties, donor-acceptor groups
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