DFT/TD-semiempirical study on the structural and electronic properties and absorption spectra of supramolecular fullerene-porphyrine-metalloporphyrine triads based dye-sensitized solar cells

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DFT/TD-Semiempirical study on the structural and electronic propertiesand absorption spectraof supramolecular Fullerene-Porphyrine-Metalloporphyrine triads based Dye-Sensitized Solar Cells

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Abstract:

In the present work density functional theory (DFT)andtime-dependent semiempirical ZNIDO/S (TD-ZNIDO/S)methodshave been used to investigate the ground state geometries, electronic structures and excited state properties of triad systems. The influences of the type of metal in the porphyrin ring, change in bridge position and porphyrine–ZnP duplicate on the energies of frontier molecular orbital and UV–Vis spectra has been studied. Geometry optimization, the energy levels and electron density of the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO), chemical hardness (η), electrophilicity index (ω), electronacceptingpower (ω^{+}) were calculatedusing ZINDO/Smethodto predict which molecule is the most efficient with a great capability to be