Electronic structure and optical properties calculation of Zn-porphyrin with N-annulated perylene adsorbed on TiO2 model for dye-sensitized solar cell applications: A DFT/TD-DFT study

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 The current work scrutinizes the chemical behavior of a set of promissory dyes, the Zn-porphyrins with N-annulated Perylene, WW3m-WW8m, within the most important steps in the solar cell: photoexcitation, electron injection and dye regeneration. The photoexcitation step was studied through TD-DFT framework, finding that the most intense band in WW4m, WW6m-WW8m corresponds to the electronic transition of the frontier orbitals HOMO-LUMO. Among these, WW6m is highlighted, because the electronic density of the LUMO is localized over the anchoring group. Therefore, the presence of two ethynylene spacers in the WW6m porphyrin originate an enhancement in the light absorption. On the other hand, we analyze the electron injection modelling two (mono and bidentate) adsorbing modes in WW3m@TiO2-WW8m@TiO2 using DFT (B3LYP+D3) calculations. Adsorption energies show that WW3m@TiO2-WW8m@TiO2 are coordinated in bidentate mode. In this sense, to analyze the density of states (DOS) w