Substituents role in zinc phthalocyanine derivatives used as dye-sensitized solar cells. A theoretical study using Density Functional Theory

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A series of zinc phthalocyanine dyes with different electron-donating and electron-withdrawing substituents and using the COOH as the anchor group that interacts with the semiconductor (TiO2) surface, were studied employing DFT and TDDFT methodologies. Their HOMO and LUMO orbital energies and, the redox mediator position would facilitate the injection process toward the conduction band of TiO2. We tested the effect of some electron-donating or electron-withdrawing substituents over zinc phthalocyanine dyes in terms of the Hammett parameters (??). We obtained a linear correlation between the substituents properties versus the free energy change of the electron-injection (?Ginject) process.