

Computational studies on the effect of introducing a π -Bridge on the efficiency of a Perylene-Brazilein based D-D- π -A systems

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ABSTRACT

We report DFT studies on some perylene based dyes for their electron transfer properties in solar cell applications. The study involves modeling of donor - donor - π - acceptor type sensitizers, with perylene and brazilein as donors and thiophene as the π -bridge. The effect of introducing a π -bridge as well as varying the π -bridges in this D-D- π -A framework was evaluated in terms of opto-electronic and photovoltaic parameters such as HOMO-LUMO energy gap, λ_{max} , light harvesting efficiency(LHE), electron injection efficiency (Φ_{inject}), excited state dye potential ($E^{\text{dye*}}$), reorganization energy(λ), and free energy of dye regeneration ($\Delta G_{\text{dye}}^{\text{Regen}}$).

All quantum computations were carried out using DFT using 6-311G(d, p) / LanL2DZ (for I and Ti atoms) as the basis sets and B3LYP as the functional, both in the gas phase as well as solvent phase, with Gaussian 03 set of codes. We found that the sensitizers exhibited good optical as well as photovoltaic response with PB2, PB7, PB8 and PB9 having benzene, pyrimidine, pyrazine and aniline as π -bridges, exhibiting better electron injection efficiencies and hence expected to be better sensitizers. The overall opto-electronic and transport parameters of the TiO₂ - dye adsorbed systems after anchoring the dyes on the model TiO₂ cluster was also studied.

Keywords: Dye sensitized solar cells; Sensitizers; Optoelectronic properties; Photovoltaic response.