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Theoretical investigation of 1,4-naphthalene dicarboxylic acid based dye-sensitized solar cells (DSSC)

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Density Functional Theory (DFT) is used to evaluate the performance of dyes and the role of π-conjugation in dye-sensitized solar cells (DSSCs). This study examines five new 1,4-naphthalene dicarboxylic acid based conjugated donor-π-acceptor (D-π-A) organic dyes. Each dye features a triphenylamine (TPA) group as the electron donor, while a nitro or cyano group serves as the electron acceptor. Methyl or ethyl groups are used as π-conjugated spacers to investigate the effects of different auxiliary donor groups. DFT calculations with the B3LYP functional and polarized split-valence 6-311+G(d,p) basis sets have been performed to assess excitation energies, absorption spectra, and emission spectra of each dye. The Polarizable Continuum Model (PCM) has been applied to analyze solvent effects. The energy levels of the LUMO and HOMO have been calculated to evaluate their suitability for electron injection and dye regeneration. The HOMO-LUMO gap calculations align well with spectral data. Additionally, the light-harvesting efficiency (LHE), electron injection free energy (ΔG_{inject}), and oscillator strength (f) have been computed and discussed. The study also includes calculations of open-circuit photovoltage (V_{oc}) and electron coupling constant (V_{RP}) for the examined dye-sensitizers.

Keywords: 1,4-Naphthalene dicarboxylic acid derivatives, Dye sensitized solar cells, Density functional theory, Light harvesting efficiency

The [illegible] of fossil fuels has led to their depletion [illegible] sensitizers because of their low cost and good