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Enhancing the optoelectronic properties of blended triphenylamine-betalain based dyes through tailoring the anchoring unit: a theoretical investigation

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Enhancing the optoelectronic properties of blended triphenylamine-betalain based dyes through tailoring the anchoring unit: a theoretical investigation

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Abstract

A series triphenyl-betalain organic dyes featuring carboxylic acid and nitro anchoring groups CH = C(X)COOH for the A1-X dyes and -CH = C(X)NO2 for the A2-X dyes, respectively, where X = CN, CH3, CCl3 and CF3 was evaluated for dye sensitised solar cells application. The geometrical structures, molecular orbitals and energies, light absorption patterns, free energies of electron injection and dye regeneration and binding to the semiconductor have been explored using DFT/TD-DFT methods. The nitro-based anchoring group resulted in pronounced red-shift in absorption spectra between 111 and 317 nm compared to carboxylic acid-based dyes. Attachment of the dyes to the semiconductor was modelled via binding to (TiO2)6H3 cluster; A2-X dyes exhibited more stable Dye@TiO2 complexes with binding energies (BEs) ranging between −4.08 and −2.88 eV compared to A1-X dyes with BEs range of −1.11 to −0.05 eV. The results evince that the dyes with CH = C(X)NO2 anchoring groups could be promising materials for light harvesting application.

Keywords; Anchoring group, DFT, betalain, triphenyl-betalain, sensitiser