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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