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New Dye Sensitizers from Anthraquinone Derivatives for Application in Dye-Sensitized Solar Cells: a DFT Study

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New dye sensitizes from anthraquinone derivatives for application in dye–sensitized solar cells (DSSCs) were theoretical investigated. The ground and excited state properties of the dyes were studied by using density functional theory (DFT) at M06/6–311G(d,p) level and time–dependent DFT (TD–DFT) method at the same level, respectively. The introduction of the anthraquinone derivatives has been shown to interestingly affect the geometrical and electronic properties of dye sensitizes for the DSSCs. In addition, effects of dyes adsorbed on surface of semiconductor TiO_2, namely dye@TiO_2, were also investigated. Moreover, thermodynamic and optical properties have been studied and reported.

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