Computational modelling on donor configuration for wide solar energy capture

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Computational modelling on donor configuration for wide solar energy capture

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Abstract

The structural and electronic properties of newly designed organic dyes have been examined by means of density functional theory (DFT) and time-dependent density functional theory (TD-DFT). The ground state molecular structures of the designed dyes are fully optimized by DFT calculation in the gas phase. Electronic absorption characteristics are predicted by the TD-DFT calculation. The calculated electronic absorbance spectrum shows red shift if the donor is doubled. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy gap were decreased. The electronic and optical properties of the donor modified sensitizers were investigated by DFT and TD-DFT methods for dye sensitized solar cell (DSSC) application.

Keywords: Solar Energy Materials; Simulation and Modelling; HOMO-LUMO; DSSC; Light Harvesting Efficiency; Density Functional Theory.

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