Acceptor Modified Influence on Tetrahydroquinoline Efficient Chromophores for Optoelectronic Properties - A First Principle Study

Govindarasu R[1] and subramanian MK[2]

[1]Thiruvalluvar Government Arts College
[2]Thiruvalluvar Government Arts College Department of Physics

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Abstract

In this study, a theoretical investigation of the photoinduced charge transfer (CT), electron injection, regeneration and Non-linear optical (NLO) of the A1-A4 structures were carried out for optoelectronic applications based on tetrahydroquinoline (C1-1) dye. Besides, a detailed assessment of the association among the electronic structures, chemical hardness, spectral and photovoltaic (PV) presentation were defined in DSSCs. Furthermore, this exploration purposes improved the electron-injection procedure, as well as the light-harvesting efficiency (LHE) of the dyes. For the research purpose, PO3H2, CONHOH, SO2H and OH (A1-A4) chromophores effects among the tetrahydroquinoline moieties related via a thiophene group were used as the electron acceptor group. The density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations were executed on the designing dye molecules. The presentation of three functional groups (Becke's three-parameter and Lee-Yang-Parr (B3LYP), coulomb-attenuating method-B3LYP (CAM-B3LYP) and Head-Gordon model (ωB97XD) were analyzed maximum absorption peak for C1-1. Here, TD-OB97XD with the 6-31G(d) combined functional and basis set were provided reliable effects to the C1-1. Therefore, newly designed A1-A4 dyes in absorption spectra were followed by TD-OB97XD method. Among these results, A1 dye displays red-shift and higher molar extinction coefficient than the other dyes and C1-1. It is specified that the PO3H2 have better PV properties, compared to literature. The NLO belongings of the A1-A4 sensitizers were derived in the polarizability and first-order hyperpolarizability. The calculated value of A1 dye has best for NLO presentation. The theoretically outcomes were intensely recommended that molecular proposal of the sensitizer has a vital role for the optoelectronic properties.

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