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Altering the UV-Vis spectra of photoactive molecules using small fragments

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The energy provided by the sun in one hour is larger than the energy consumption globally each year thus it has been a challenge to convert solar energy to electricity cost-effectively in organic dye sensitized solar cells (DSSC). In recent years photoactive molecules such as the most recently available zzx-op dyes have gained attention due to their potential to construct high efficiency tandem cells with conventional n-DSSCs. A number of high performing p-type push and pull dyes, i.e., zzx-op dyes which consist of a perylenemonoimide (PMID) as an electron acceptor (A) and a di(p-carboxyphenyl)amine (DCPA) as an electron donor (D) and a pi-conjugated linker for the D-pi-A dyes are recently synthesized. In this presentation, we focus on the expansion of the UV-Vis spectra of these photoactive molecules through rationally change the pi-linkers through molecular modelling by combining their optimal combinations which best enhance the UV-Vis spectra of the new photoactive molecules (Fig. 1). Time-dependent Density functional theory (TD-DFT) simulation using DFT based PBE0/6-311G(d) model are employed to simulate the UV-Vis spectra. The results have shown in the improvement of the UV-Vis absorption and preliminary results will be presented.

Keywords

P-type, DSSC, NiO, PUSH PULL DYES

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