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Investigation of optoelectronic properties of triphenylamine-based dyes featuring heterocyclic anchoring groups for DSSCs' applications: a theoretical study

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Abstract

Design and synthesis of new potent sensitizers are of interest for realization of high-efficiency Dye Sensitized Solar Cells (DSSCs). Modification of the triphenylamine-based dyes by introducing suitable anchoring groups aimed at improvement of optoelectronic properties is attempted in our work. The molecular structure, molecular orbitals and energies, electronic absorption spectra, free energies of electron injection and dye regeneration, chemical reactivity parameters and adsorption to TiO2 semiconductor have been reported. Density functional theory (DFT) and time-dependent DFT (TD-DFT) were used to obtain the reported properties. The results reveal superior optical, electronic properties, chemical reactivity parameters and adsorption energies for the investigated dyes. The findings evince that the dyes featuring heterocyclic anchoring groups could be potential candidates for DSSCs' applications; the new materials are worthy of being investigated experimentally.

Keywords

Anchoring groups; TD-DFT; Heterocyclic; TPA-based sensitizers