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Tuning optoelectronic properties of diphenylamine based dyes through variation of pi-conjugated units and anchoring groups: A DFT/TD-DFT investigation

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Abstract

Dye-sensitized solar cells (DSSCs) have attracted widespread attention due to their unique features. In the present work, molecular engineered triphenylamine based dyes featuring donor-bridge-acceptor architecture have been considered and investigated for suitable properties for DSSCs applications. Hydantoin anchoring group has been introduced replacing the commonly used cyanoacrylic acid to improve the long-term stability of the device. Results on the effects of varied anchoring groups and pi-spacers have been interpreted from the viewpoint of DFT/TD-DFT calculations. Designed sensitizers exhibit suitable light-harvesting efficiencies, excited-state lifetimes, electron injection and regeneration abilities. Red-shifted electronic spectra are observed for three hydantoin dyes compared to others in the same family. Further analysis of chemical descriptors and observation from full-electron donor-acceptor map reveal that the three dyes among nine are potential materials with promising properties towards improving DSSCs performance.

Keywords

Cyanoacrylic; DSSC; Hydantoin; Optoelectronics; Triphenylamine