Experimental and theoretical analysis of organic dyes having a double D-π-A configurations for dye-sensitized solar cells

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Abstract

Two spiro-like organic dyes linked at the thiophene bridge (KS-11 and KS-12) together with the original rod-shaped D-π-A configuration (C1) were designed, synthesized, and characterized based on their electronic structure, and determine the photophysical and photovoltaic properties for its application in dye-sensitized solar cells. Compared to C1, the double D-π-A spiro-like configuration, which consists of two separated light-harvesting moieties, was found to be beneficial to photocurrent generation provided that they are separated properly to prevent intramolecular exciton annihilation. This was observed when KS-11, which is linked at the β-position of the thiophene moiety of D-π-A, was compared with KS-12, where the two D-π-A are linked with an additional thiophene using a α-β linkage. The results show that KS-12 produced a 20% and 17% increase in photovoltaic efficiency under simulated AM 1.5G solar irradiation compared to KS-11 and C1, respectively. This increase in photovoltaic performance is credited mostly to the reduction of recombination effects and the increase in the density of states at the semiconductor surface due to high dye loading and better charge-transfer properties.

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