

Effects of heterocyclic ring and amino-ethyl-amino group on the electronic and photophysical properties of a triphenylamine-pyrimidine dye

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Abstract

Introduction of a heterocyclic ring and an amino-ethyl-amino group to D-A type photosensitive dyes can modulate the lifetime of the charge separation generated in the D-A dyes as well as their electronic and UV-Vis absorption properties. Here we performed DFT and TDDFT calculations to study eleven derivatives of a triphenylamine-pyrimidine, MTPA-Pyc, in order to improve the performance of MTPA-Pyc as solar cell sensitizers. Five heterocyclic rings and an amino-ethyl-amino group were introduced on the styryl moiety of MTPA-Pyc. The results show that introduction of heterocyclic rings generally causes an absorption red-shift, but absorption intensity is reduced due to the increase of dihedral angle between the donor and acceptor. Further introduction of an amino-ethyl-amino group to these dyes with a heterocyclic ring modification disrupts the conjugation between donor and acceptor, which does not benefit the absorption but may have potential to increase the lifetime of charge separation of the dyes. This work identified two out of eleven dyes that have the best potential for solar cell applications.

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