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Communication

Organic dyes containing fused acenes as building blocks: Optical, electrochemical and photovoltaic properties

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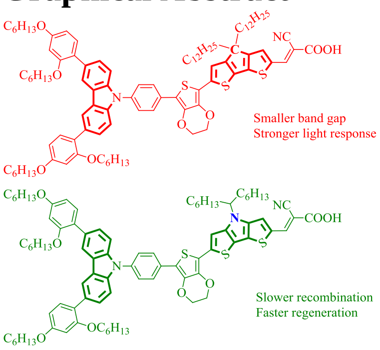
Graphical Abstract



ABSTRACT
Two D-π-A dyes based on fused acenes (carbazole, cyclopenta[2,1-b:3,4-b']dithiophene (CPDT) and dithieno[3,2-b:2',3'-d]pyrrole (DTP)) were synthesized, characterized using UV-vis absorption spectroscopy and electrochemistry, density function theory (DFT) calculations, and used as sensitizers in dye-sensitized solar cells (DSSCs). The two sensitizers were compared thoroughly over physicochemical properties and DSSC performance. Although the DTP dye has slightly blue-shifted and weaker incident photon-to-collected electron (IPCE) conversion efficiency responses, the much increased open-circuit photovoltage values and improved charge-transfer kinetics relative to the CPDT systems result in superior power conversion efficiencies. This work reveals the potential of DTP as a bridge in the design of sensitizers.

Keywords:
Dye-sensitized solar cells
Fused acene
D-π-A
9-Phenyl carbazole
Dithienopyrrole

Dye-sensitized solar cell (DSSC), since it was firstly reported in 1991 by O'Reagan and Grätzel [1], initiated the possibility of maximizing the harnessing of solar light in a cost-efficient way. The principle of the DSSC is based on a broadband inorganic semiconductor scaffold, *e.g.*, TiO_2, which is sensitized with a strongly absorbing dye. High efficiencies up to 13% have been achieved by employing a meso-substituted porphyrin dye in conjunction with a tris(2,2'-bipyridine)cobalt(II/III)redox couple [2]. Recently, Hanaya *et al.* [3–5] developed a collaborative sensitization strategy combining ADEKA-1 and LEG4 dyes in DSSC with silyl-anchor and carboxy-anchor respectively. They realized a high light-to-electric power conversion efficiency (PCE) of over 14.5% under one sun illumination due to successful pinhole filling by dye layers with multiple coadsorbates to reduce interfacial charge recombination.

Among the five key components of DSSC: Transparent conductive oxide such as fluorine-doped SnO_2 (FTO), mesoporous semiconductor metal oxide (such as nanocrystalline TiO_2), sensitizer (dye), electrolyte/hole transporter, and counter electrode (platinum or carbon on FTO), the dye takes up a big fraction of the total cost. Despite the excellent light harvesting ability, the tedious synthesis of porphyrin dyes labels itself as a luxurious choice for DSSC community. In the meantime, the easily accessible metal-free organic dyes based on arylamines especially triphenylamine (TPA) (Fig. 1) as electron donating fragments have shown excellent electronic properties [6–14].

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