Rational design of different π-bridges and their theoretical impact on indolo[3,2,1-jk] carbazole based dye-sensitized solar cells

ABSTRACT

Eight new π-bridges for a promising indolo[3,2,1-jk] carbazole based dye IC-2 were rationally designed. In the first set of derivatives, π-bridges consisting of thiophene, furan and pyrrole ring were constructed. The bridges were then extended with additional heterocyclic ring linked together with either ethylene or azo moiety. Their structural, electronic, optical and photovoltaic properties were evaluated based on density functional theory calculation. π-Bridges containing furan ring and azo moiety were the most planar and demonstrated smaller HOMO and LUMO gap. Extended furan π-bridge with azo group exhibited the lowest excitation energy and broadest UV-Vis absorption peaks. Large values of the light harvesting ability were observed for all extended π-bridges while pyrrole π-bridges resulted in the highest value of open circuit voltage. Based on these properties, the extended compounds would be good candidates for DSSC and further investigation on dye@TiO2 complex systems is warranted.