Highly efficient dye-sensitized solar cells using simple phenothiazine-based dyes

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**Abstract**

The unique structural features of phenothiazine-based dye make it a promising type of sensitizers for dye-sensitized solar cells (DSSCs). Recently, a diversity of strategies have been utilized to extend the range of π-electron delocalization and increase the molar absorptivity of the materials. In our studies, we designed and synthesized a series of slim phenothiazine-based dyes for DSSCs, in which a cyanoacrylate acceptor directly attached to the C(3) position of phenothiazine, and an additional linear electron-rich group at C(7) on the opposite side of the acceptor, and an alkyl chain with different length at N(10) of the phenothiazine periphery are presented. The dye molecules have a slim shape which is favorable for the formation of a compact dye layer on the $TiO_2$ surface, while their butterfly conformations can sufficiently inhibit molecular aggregation (Figure 1). Moreover, the structural features of aryl donor moiety at the C(7) position of phenothiazine extends the π-conjugation of the chromophore, thus enhancing the performance of DSSCs. Moreover, the alkyl substituents with different chain length at the N(10) atom of phenothiazine could further optimize the performance through completely shielding the surface of $TiO_2$ from the $I^-/I_3^-$ electrolyte and subsequently reducing the leakage of dark current. Under simulated AM 1.5G irradiation, the best DSSC performance shows a short-circuit photocurrent of 15.32 mA cm-2 , an open-circuit photovoltage of 0.78 V, a fill factor of 0.69, corresponding to a power conversion efficiency (PCE) of 8.18%, which exceeds the reference N719 (7.73%) under identical fabrication conditions. Notably, the designed molecular structure represents the highest photovoltaic conversion efficiency value when compared with other reported phenothiazine-derived dyes.

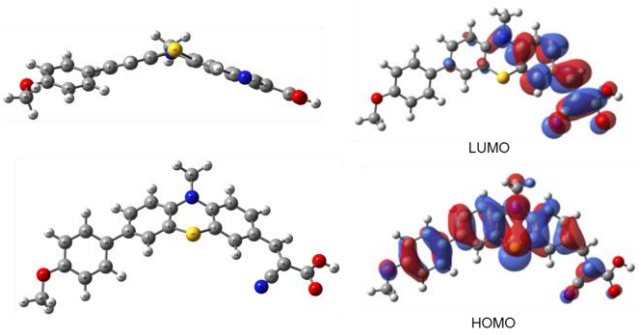


Figure 1. Optimized ground state geometry (left) and frontier molecular orbitals of the HOMO and LUMO (right) calculated by DFT on a B3LYP/6-31 t G (d)* level.