Theoretical Study on Linker Type Effect in the Perylene bisimide Based Dyes for Dye-Sensitized Solar Cells

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Abstract

A series of newly synthesized organic donor–π–acceptor dyes are theoretically studied and compared with our experimental measurements. These dyes are based on Perylene bisimide and cyanoacrylic acid moieties as donor and acceptor units, respectively. By using density functional theory (DFT) and time-dependent DFT (TD-DFT) methods, we have investigated their potential performances in dye-sensitized solar cells (DSSCs). Effects of different π-linkers in these dyes on the energy conversion efficiency of the DSSCs are investigated through optimized geometries, electronic structures, absorption spectra, and free energies of injection. The calculated results show that the molecular orbital energy levels and electron-injection driving forces of the dyes can be tuned by the variation of π-linkers with different electron transporting abilities. By analyzing the light-harvesting efficiencies and the free energies of injection, we can predict the trend of DSSCs performances based on these dyes which are consistent to our experimental observations. PThTA dye having thieno[3,2-b]thiophene as the liker exhibits highest efficiency in DSSCs among the studied dyes.

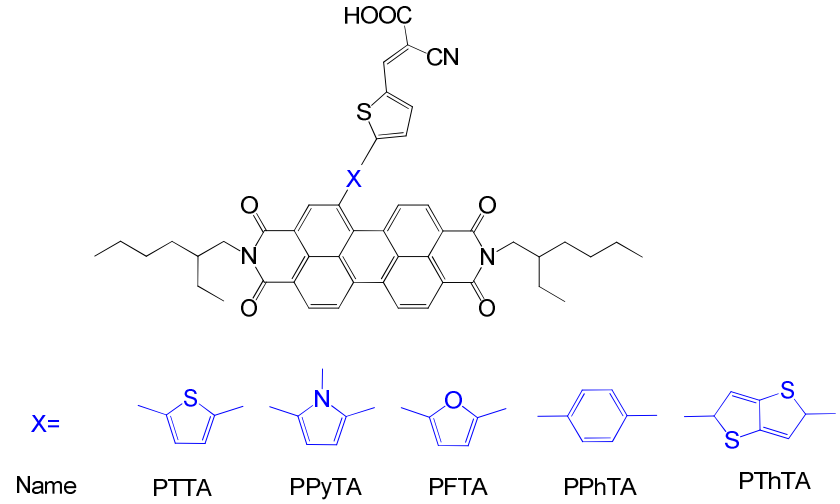

Figure. Sketch map of the studied dyes.

Keywords: DFT, TDDFT, Perylene Bisimide, Dye-sensitized Solar Cells