Study on the Electron Injection of Newly Synthesized Organic Sensitizer in Dye-Sensitized Solar Cell

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Electronic and photovoltaic characteristics of two sensitizers (TA-BTD-CA and TA-BTD-St-CA), composed of a different π-conjugation in the linker group, have been investigated by theoretical and experimental methods. The electronic structure, transition dipole moment and oscillator strengths of two sensitizers have been scrutinized by using density functional theory (DFT) and time-dependent DFT (TD-DFT) method. The LUMO level and the oscillator strength of TA-BTD-St-CA was higher than that of TA-BTD-CA, which may facilitate the electron injection process as well as increase the absorption coefficient. The relative efficiencies of the electron injection from the excited sensitizer to nanocrystalline TiO2 and SnO2 films have also been investigated by nanosecond transient absorption spectroscopy. The relative electron injection efficiency of TA-BTD-St-CA exhibited similar injection efficiency for two different semiconductors. However, in the case of TA-BTD-CA sensitizer, electron injection into SnO2 was approximately three times larger than that into TiO2. This enhancement of electron injection of TA-BTD-CA for the SnO2 is due to the increment of the driving force caused by positive shift of conduction band of semiconductor, which was also confirmed from the investigation for the photovoltaic characteristics according to the electrolyte additive, such as LiI additive.