Charge Transport in Nanocrystalline TiO_2 films of Dye-sensitized Solar Cells

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Dye-sensitized solar cells (DSCs) are composed of a dye-coated nanocrystalline TiO_2 film on a transparent conductive oxide (TCO) glass, an electrolyte solution containing triiodide/iodide (I_3^-/I^-) redox couple, and a counter electrode (See Fig. 1). The nanocrystalline films consist of interconnected nano-particles (10-30 nm) act as a high surface area for dye adsorption. The electrolyte solution permeates into the nano-pore. Under illumination, excited dyes rapidly inject electrons into TiO_2. The injected electrons are transported to TCO glass through the nanoporous TiO_2. The dyes are regenerated from their oxidized states by I_3^-/I^- redox couple. The I_3^-/I^- redox couple also have to be transported in nano-pore of TiO_2.

According to electron transport, an electric field of nanoporous TiO_2 is neutralized by many ions in the electrolyte solution since the electrolyte solution also contains numerous counter cations such as Li^+ and imidazolium ions for I_3^-/I^- redox couple [2,3]. Therefore, the electron transport is dominated by a gradient (diffusion) of electron density in nanoporous TiO_2 rather than by an electrical potential gradient (drift). The photovoltaic performance has been explained by the electron diffusion model. However, the electron diffusion model cannot clearly explain the electron density (irradiation power) dependent diffusion coefficient. The viscosity of an electrolyte solution, the concentration of I_3^-/I^- redox couple, and other counter cations also influence on the photovoltaic performance. Recently, we also have found that the dyes on TiO_2 also influence on the charge transport [3]. The charge transport mechanism including the transport of electron and I_3^-/I^- redox couple will be presented.

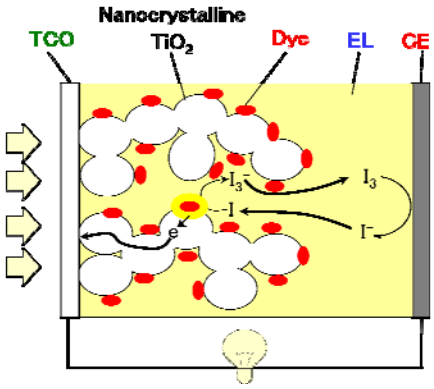

Fig.1 Schematic of dye-sensitized solar cells.
TCO is a transparent conductive oxide, EL is an electrolyte solution, and CE is a counter electrode.

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Tuning of HOMO and LUMO energy level of Ru(II) terpyridyl sensitizers to enhance light-harvesting properties of dye sensitized solar cells (DSCs)

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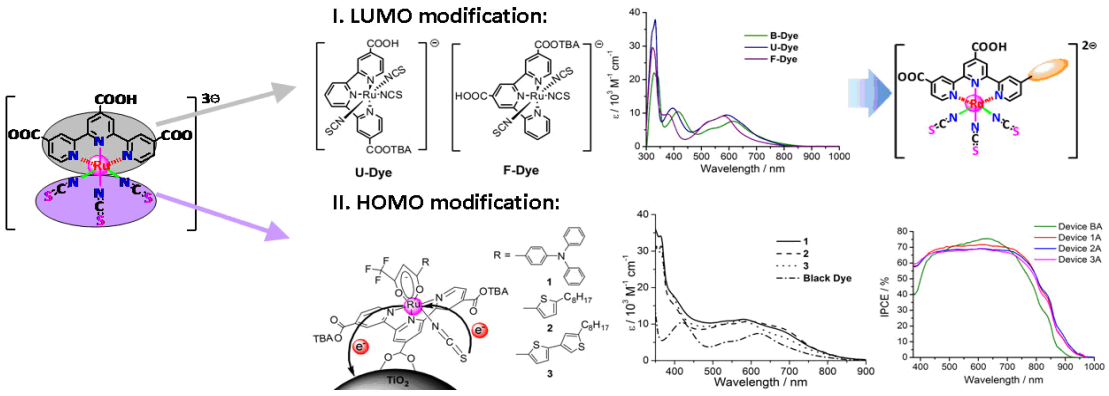
Dye-sensitized mesoscopic TiO_2 solar cells (DSCs) have attracted a growth of interest because of their high photon-to-electricity conversion efficiency and low production and material cost during the past two decades. In this device, the sensitizer has been recognized as one of the key components for high cell performance. The most efficient sensitizers employed so far in DSCs are Ru(II) polypyridyl complexes because of their broad and intense metal-to-ligand charge transfer (MLCT) absorption in the whole visible range. To further improve the conversion efficiency, an enhanced light-harvesting capability of the sensitizer in lower energies is required. Systematic tuning of the LUMO and HOMO moieties of the Ru(II) polypyridyl complexes is successful strategy to fulfill the above target.

Herein, we resent our efforts in the molecular engineering of Ru(II) terpyridyl complexes. (1) Utilizing the *β*-diketonato ligands with different donor-conjugated antennas to substitute the NCS groups to act as the HOMO moieties;[1] (2) Developing new terpyridyl ligands to act as the LUMO moieties. The synthesis, physical and photovoltaic properties of the newly developed sensitizers will be presented.



[1] Shang Gao, Ashraful Islam, Youhei Numata, and Liyuan Han, Applied Physics Express 3 (2010) 062301.