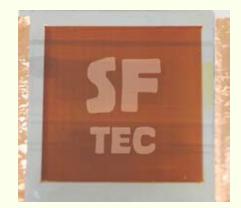


DSSC Dye sensitized solar cells

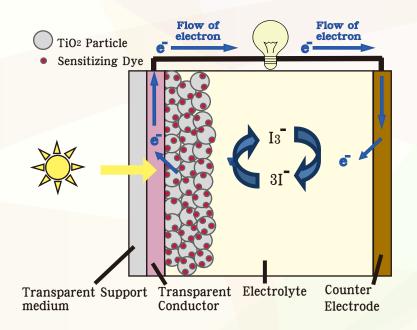


Organic Dye Ruthenium Complex Dye

DSSC Dye sensitized solar cells

Dye sensitized solar cells are a new kind of photovoltaic devices; they can reach an efficiency higher than 10% and have great potential for providing low-cost photovoltaic power; in fact these cells can be produced easily without the expensive set-ups needed for conventional solid-state solar cells.

The system comprises a dye that is bound to the surface of an inorganic semiconductor. Typically nanocrystalline TiO2 is used as it provides a large surface area to which the dye can adsorbs, which is crucial for efficient light harvesting. The porous TiO2 layer is interpenetrated by a hole-transport material (HTM), which may be a oxidation-reduction electrolyte in solution or a solid-state or quasi-solid-state (gel) material.



Chemical reaction involved:			
Anode (working electrode) :	$S + h v \to S^{\star}$	Absorbtion	
	$S^{\star} \rightarrow S\text{+} \text{+} \text{e-} (\text{TiO2})$	Percolation	
	$2S++3I- \rightarrow 2S+I3-$	Regeneration	
Cathode (counter-electrode) : I3- + 2e- (Pt) \rightarrow 3I-			
Cell:	e- (Pt) + hv \rightarrow e- (TiO2)		

Excitation of the dye leads to the injection of electrons from the excited dye to the conduction band of the TiO2. The ground state of the dye is regenerated through reduction by the HTM to give the required charge separation. Charges migrate and are collected at a transparent conducting electrode (electrons) and Pt electrode (holes).



DSSC Dye sensitized solar cells

ACTIVITIES

TiO2 anatase nanocrystals synthesis and mesoporous TiO2 film preparation

A high light-to-electricity conversion efficiency results from a large surface area of porous TiO2 electrodes, on which the dyes can be sufficiently adsorbed. The thickness of mesoporous TiO2 films should be about 10 µm.

The overall mechanism involves light absorption by the dye, resulting in rapid electron injection into the conduction band of the semiconductor.

The role of the titanium dioxide thin film is crucial and the cells efficiency strongly depends on the surface and electronic properties of the semiconductor. Some important features that TiO2 mesoporous films should possess are:

- extremely large surface area, necessary to achieve extended chemisorption of dye molecules,
- interconnection and continuity between nanosized titania nanoparticles to avoid charge carrier accumulation, achieve efficient electron flow and finally assure current collection at the back contact of the photoelectrode,
- solid structure of the film (absence of cracks or other surface defects) resulting in rapid and highly efficient interfacial charge transfer,
- porous structure permitting extended interaction of the electrolyte with the oxidized dye molecules and therefore efficient regeneration of Ru(II) dye.

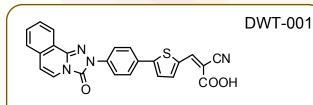
Dye synthesis

Ruthenium dyes are normally used in dye-sensitized solar cells and exhibit high performance and good stability. However, Ru dyes are very expensive due to the rarity of the metal. Some metal-free organic dyes are shown to be promising sensitizers for nanocrystalline solar cells in view of their properties such as high absorption efficiency and their low cost. They must bind strongly to TiO2 by means of an anchoring group, typically carboxylic or phosphonic acid groups, to ensure efficient electron injection into the TiO2 conducting band and to prevent gradual leaching by the electrolyte. The LUMO of the dye must be sufficiently high in energy for efficient charge injection into the TiO2, and the HOMO must be sufficiently low in energy for efficient regeneration of the oxidized dye by the HTM. They should contain a structure with donor-to-acceptor moieties bridged by a π -conjugation unit.

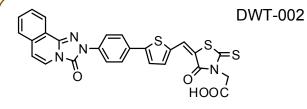




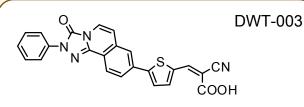
Organic Dye



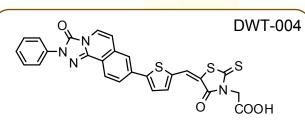
(2Z)-2-cyano-3-(5-(4-(3-oxo-[1,2,4]triazolo[3,4-a] isoquinolin-2(3H)-yl)phenyl)thiophen-2-yl) acrylic acid



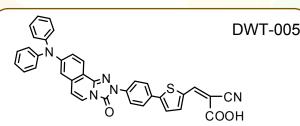
2-(5-(4-(3-oxo-[1,2,4]triazolo[3,4-a]isoquinolin-2(3H)-yl)phenyl)thiophen-2-yl)methylene)-4-oxo-2-thioxothiazolidin-3-yl)acetic acid



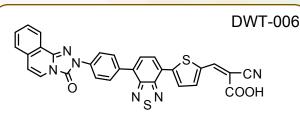
(2Z)-2-cyano-3-(5-(2,3-dihydro-3-oxo-2-phenyl-[1,2,4]triazolo[3,4-a]isoquinolin-8-yl)thiophen-2-yl) acrylic acid



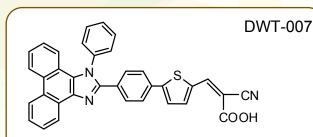
2-(5-(2,3-dihydro-3-oxo-2-phenyl-[1,2,4]triazolo [3,4-a]isoquinolin-8-yl)thiophen-2-yl)methylene)-4oxo-2-thioxothiazolidin-3-yl)acetic acid



(Z)-2-cyano-3-(5-(4-(8-(diphenylamino)-3-oxo-[1,2,4] triazolo[3,4-a]isoquinolin-2(3H)-yl)phenyl)thiophen-2-yl)acrylic acid

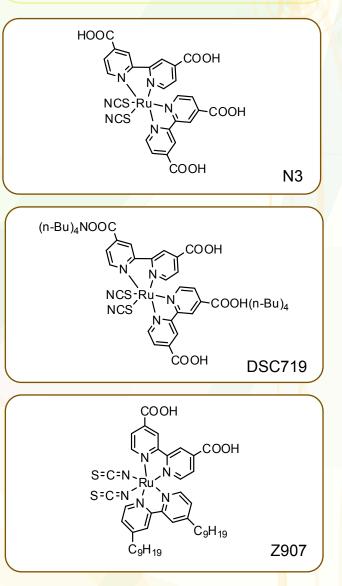


(Z)-2-cyano-3-(5-(7-(4-(3-oxo-[1,2,4]triazolo[3,4-a] isoquinolin-2(3H)-yl)phenyl)benzo[c][1,2,5]thiadiazol -4-yl)thiophen-2-yl)acrylic acid



(Z)-2-cyano-3-(5-(4-(1-phenyl-1H-phenanthro[9,10d]imidazol-2-yl)phenyl)thiophen-2-yl)acrylic acid

Ruthenium Complex Dye



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