

Supplementary Information

Efficient Flexible Dye-Sensitized Solar Cell with a Photoanode Consisting of
TiO₂ Nanoparticles-Filled and SrO-Coated TiO₂ Nanotube Array

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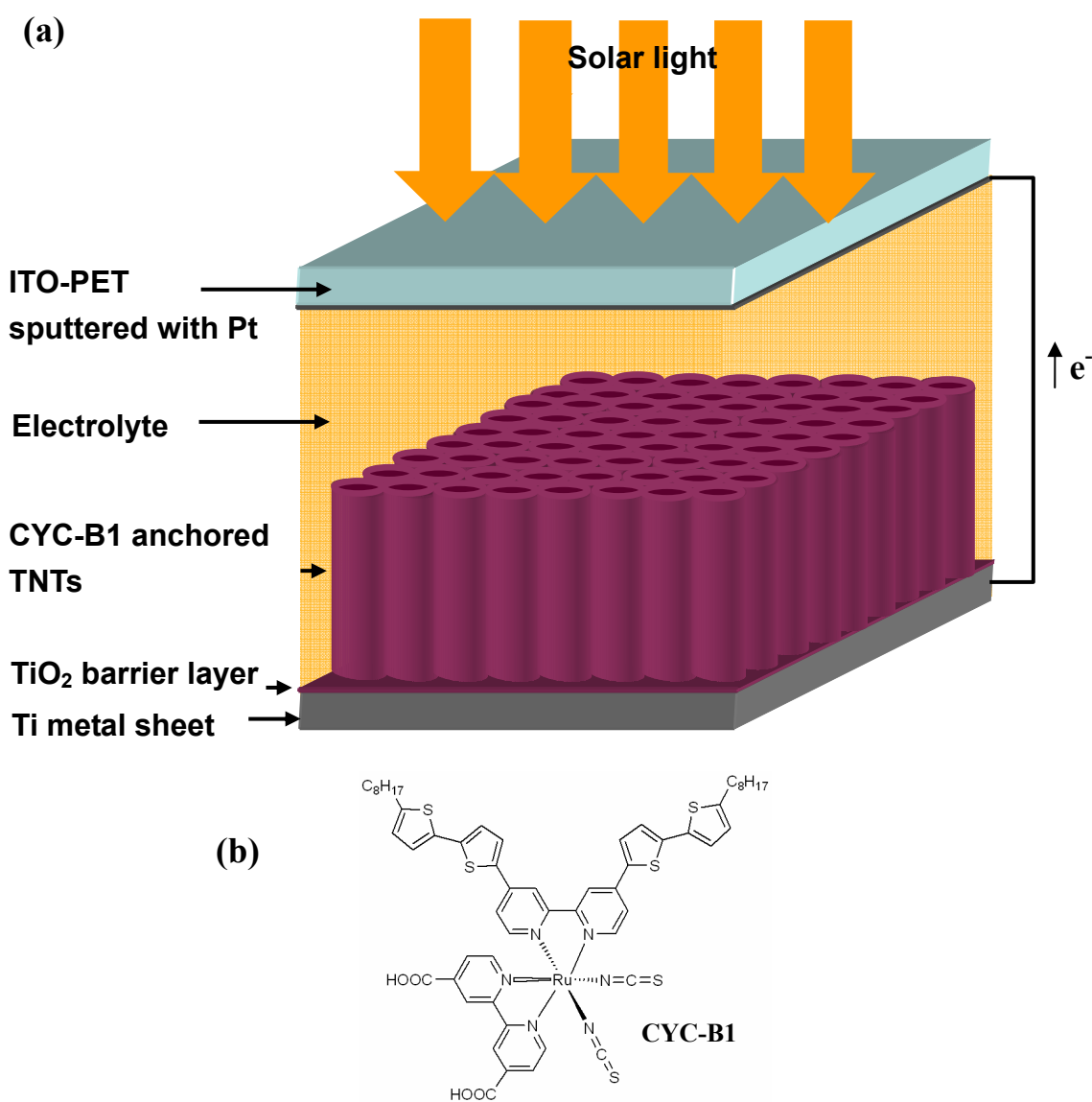


Figure S1 (a) Schematic diagram of the back-illuminated DSSC with arrays of TNT as the photoanode, (b) chemical structure of CYC-B1 dye.

Mott-Schottky-plots analysis

The Mott-Schottky-plots analysis predicts a linear relationship between the applied potential and the inverse square of capacitance ($1/C_{sc}^2$) arising from the space charge layer in a semiconductor.¹ Under biasing conditions where the semiconductor space charge region is in depletion, capacitance of the space charge region can be obtained by the following equation,

$$\frac{1}{C_{sc}^2} = \frac{2}{e\epsilon_0\epsilon N_d} \left(-\Delta\phi - \frac{kT}{e} \right) \quad (1)$$

here e is electronic charge (1.6×10^{-19} C), ϵ_0 is the permittivity of free space (8.86×10^{-12} F/m), ϵ is the dielectric constant of the TiO_2 , N_d is dopant (donor or acceptor) concentration, $-\Delta\phi$ is the difference between the applied potential and the flat-band potential ($E - E_{fb}$), k is the Boltzmann constant, and T is the absolute temperature.²

Considering the fact that the term of kT/e is 0.026 eV at room temperature, which was insufficient to influence the original value, equation (1) may be briefly rewritten as follow,

$$\frac{1}{C_{sc}^2} = \frac{2}{e\epsilon_0\epsilon N_d} (E - E_{fb}) \quad (2)$$

The slope of C_{sc}^2 vs. $\Delta\phi$ is inversely proportional to the effective donor or acceptor concentration in the semiconductor, and the flat-band potential can be determined by extrapolating C_{sc}^2 to 0.³ The flat-band potentials of TNT, TNT-TNP, and TNT-TNP-SrO electrode estimated from Fig. 9 (in the article), were -0.69, -0.69 and -0.73 V vs. Ag/AgCl (in saturated KCl), respectively. The data shown that the V_{fb} of the TNT-TNP-SrO electrode is more negative to those of the other two electrodes by 0.04 V. TiO_2 coated with a layer of wide-band gap material, i.e., SrO, built an inherent potential barrier layer to block electron transfer from the conduction band or trap sites of the TiO_2 to the triiodide ions of the redox electrolyte. This barrier layer enabled TNT-TNP-SrO-DSSC to have a higher V_{oc} than those of TNT-DSSC and TNT-TNP-DSSC. Using equation (2) with a linear fitting method and the physical constants of the TiO_2 material, the donor concentrations of TNT, TNT-TNP, and TNT-TNP-SrO electrodes were calculated to be 1.06×10^{16} , 1.38×10^{16} , and 2.21×10^{16} cm^{-3} , respectively. The potential barrier of SrO retards the recombination of photo-injected electrons with I_3^- ions and thereby increases the electron concentration in TiO_2 , which also contributes for a higher J_{sc} as observed in Fig. 7 (in the article). Benefited by a higher V_{oc} , J_{sc} , and FF, the TNT-TNP-SrO-DSSC showed the highest η amongst the three types of DSSC studied in this article.

Reference

- (1) E. Barsoukov, J. R. Macdonald, *Impedance Spectroscopy Theory, Experiment, and Applications*; Wiley: NJ, **2005**; Chapter 4.
- (2) G. Wang, Q. Wang, W. Lu, J. Li, *J. Phys. Chem. B*, 2006, **110**, 22029.
- (3) F. Fabregat-Santiago, G. Garcia-Belmonte, J. Bisquert, P. Bogdanoff, A. Zaban, *J. Electrochem. Soc.*, 2003, **150**, E293.