Supplementary Material (ESI) for Chemical Communications

Suporting Information - A novel blue dye for near-IR "dye-sensitised" solar cell applications

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Solid state devices: After cleaning the F-doped SnO_2 glass substrates (with acetone, methanol and Helmanex), a ~100 nm compact layer of TiO_2 was deposited by spray-pyrolysis. A nanoporous TiO_2 layer was fabricated via doctor-blading a TiO_2 paste containing 19 nm-sized anatase particles, followed by sintering at 450 °C. A 0.02 M aqueous $TiCl_4$ solution was deposited overnight on the TiO_2 films and the substrates rinsed with water. Prior to dye uptake, the substrates were annealed at 450 °C for 15min. They were sensitized by soaking in a $2.5x10^{-4}$ M solution of B1 in ethanol at room temperature. After soaking in the dye solution, the substrates were rinsed with acetonitrile. The hole transporter matrix was applied by spin coating a solution of the hole-conductor in chlorobenzene (0.17 M), containing $Li[CF_3SO_2]_2N$ (13 mM), tert.-butylpyridine (*t*BP) (0.13 M) and $N(PhBr)_3SbCl_6$ (0.3 mM). Before spin-coating, this solution was deposited onto the "dye-sensitised" substrate and was allowed to penetrate into the pores of the TiO_2 layer for one minute. To finish the device production, a 30 nm Au electrode was evaporated on top.

Liquid cell devices: The working electrodes were made from FTO glass (Nippon Sheet Glass Solar 4 mm thick). The electrodes were cleaned for 15 min in a detergent solution using an ultrasonic bath and then rinsed with water and ethanol. A compact layer of ~100 nm TiO_2 was deposited by spray-pyrolysis. The plates were immersed in a 40 mM aqueous $TiCl_4$ *aq.* solution at 70 °C for 30 min and washed with water and ethanol. A layer of paste A[21)] was coated on the FTO glass plates by screen printing (90T, Estal Mono, Schweiz. Seidengazefabrik AG Thal) and then dried for 6 min at 125 ˚C. The screen-printing procedure with paste A was repeated to get an appropriate thickness of 12 μm for the working electrode. After drying at 125 ˚C the 4 μm scattering layer was deposited by screen printing using paste B[21)]. The electrodes were heated to 325 °C for 5 min, 375 °C for 5 min, 450 °C for 15 min and 500 °C for 15 min. The films were again treated with a 40 mM $TiCl_4$ sol., rinsed with water and ethanol and sintered at 500 °C for 30 min. After

cooling (80 °C), the TiO_2 electrodes were immersed in a $2.5x10^{-4}$ M dye sol. containing $2.5x10^{-3}$ M chenodeoxycholic acid in ethanol at room temperature for sensitizer uptake.

To prepare the counter electrode, a hole was drilled in the FTO glass (LOF Industries, TEC 15Ω, 2.2 mm) via sand blasting. The glass was washed with H_2O and a 0.1 M HCl sol. in ethanol and sonicated in acetone for 10 min. The plates were heated for 15 min at 400 °C with a drop of H_2PtCl_6 solution to deposit the Pt catalyst. The photoelectrode and Pt-counter electrode were sandwiched and heated together with a 25 μm Surlyn 1702 (Dupont) ring. A drop of the electrolyte, a sol., 0.60 M BMII, 0.05 M I_2, 0.5 M TBP, 0.10 M LiI in of acetonitrile and valeronitrile (volume ratio: 85:15), was introduced via vacuum backfilling through the hole. The hole was sealed using 35 μm film (Bynel 4702, Du-Pont) and a 0.1 mm cover glass. To improve the electrical contact, solder (Cerasolza, Asahi Glass) was applied to each side of the exposed FTO electrodes.

Photovoltaic measurements employed an AM 1.5 solar simulator equipped with a 450 W xenon lamp (Model No. 81172, Oriel). The power of the simulated light was calibrated by using a reference Si photodiode equipped with an IR-cutoff filter (KG-3, Schott) in order to reduce the mismatch in the region of 350-750 nm between the simulated light and AM 1.5 to less than 2 %.[22, 23)] To prevent an over estimation of the energy conversion efficiency a mask was used with an area of 0.158 cm^2. J-V curves were obtained by applying an external bias to the cell and measuring the generated photocurrent with a Keithley model 2400 digital source meter.