

Electronic Supplementary Information for

A simple and effective crystal growth inhibitor for high performance solid-state dye-sensitized solar cells

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1. Device fabrication

The fabrication of DSSCs is fabricated as follows [S1,S2]. The FTO glass was cleaned by acetone and ethanol successively. Then, cleanly FTO glass was immersed into 40 mM aqueous TiCl_4 solution at 70 °C for 30 min and washed with water and ethanol. Firstly, a 10 μm -thick film of 20 nm-sized TiO_2 particles was coated onto the FTO glass by the doctor-blade technique and then dried at 125 °C for 5 min. Secondly, a 5 μm -thick layer of 200 nm light-scattering TiO_2 particles was deposited on the top of the first TiO_2 layer. The two layers of TiO_2 particles were used as photo anode. The resulting TiO_2 films were annealed at 500 °C for 30 min and gradually cooled to 90 °C. The obtained TiO_2 electrode was soaked in a Z907 solution (0.5 mM) containing CDCA with a molar ratio of 1:1 in acetonitrile/tert-butyl alcohol (1 : 1, v : v) for 24 h. Afterward, the dye-sensitized TiO_2 electrode was washed with anhydrous ethanol and dried with a N_2 stream. To prepare the Pt counter electrode, one drop of 5 mM H_2PtCl_6 in ethanol was dipped onto the cleaned FTO glass substrate, followed by dried and annealed at 400 °C for 15 min.

DSSCs were fabricated by sandwiching the solid-state electrolyte between a dye-sensitized TiO_2 electrode and a Pt counter electrode. The employed solid-state electrolytes A-C for Devices A-C contains EMII/10wt% I_2 , EMII/20wt%EMIBF₄/10wt% I_2 and EMII/20wt%[TMImB][Br]/10wt% I_2 , respectively. While the electrolyte B with EMIBF₄ is used for reference device. The methanol solution of the solid-state electrolytes was injected into the sandwiched cells using a vacuum

backfilling system. The cells were heated to 80 °C under vacuum to remove methanol and air from the electrolyte. This procedure was repeated several times to remove the residual methanol to guarantee optimal filling and fine electrical contact overnight. The produced devices were sealed with a Surlyn sheet and a thin glass cover by heating.

2. Characterization and Photovoltaic Measurements

¹HNMR spectra were carried out on a Varian 400 MHz spectrometer. Fourier transform infrared (FTIR) spectra of the synthesized compounds were recorded on a Varian CP-3800 spectrometer in the range of 4000-400 cm⁻¹. Thermal analysis was carried out on Universal Analysis 2000 thermogravimetric analyzer (TGA). Samples were heated from 50 to 500 °C at a heating rate of 10 °C min⁻¹ under a nitrogen flow. Differential scanning calorimetry (DSC) measurements were performed under a nitrogen atmosphere with a heating rate of 10 °C min⁻¹ in a temperature range of -50–150 °C on DSC-Q200. The viscosity measurements were performed on a viscometer (Haake® Rheo Stress 6000, Germany). Surface morphologies were investigated by SEM (Hitachi SU8010) at an accelerating voltage of 5 kV. The conductivity of the electrolytes was characterized in an ordinary cell composed of Teflon tube and two identical stainless steel electrodes (diameter of 1 cm) on a CHI660c electrochemical workstation, using the AC impedance method over the frequency range 0.1 Hz to 10⁵ Hz and the amplitude is 10 mV. The conductivity was calculated using the following equation:

$$\sigma = \frac{l}{RS} \quad (1)$$

where σ is the conductivity in S cm⁻¹, R is the ohmic resistance of the electrolyte, l is the distance between two electrodes, and S is the area of the electrodes [S2]. All the samples were equilibrated for at least 30 min at a given temperature. The photocurrent density-voltage (J-V) curves of the assembled DSSCs shielded by an aluminum foil mask with an aperture area of ~0.25 cm² were measured with a digital source meter (Keithley, model 2612) under simulated air mass (AM) 1.5 solar spectrum illumination at 100 mW cm⁻², respectively. The incident photocurrent conversion efficiency (IPCE) plotted as a function of excitation wavelength was recorded under the irradiation of a Xenon lamp with a monochromator (Oriel Cornerstone™ 260 1/4). The photoelectrochemical parameters, such as open-circuit voltage (V_{oc}), short-circuit photocurrent density (J_{sc}), fill factor (FF) and power conversion efficiency (PCE), were listed and calculated

according to the previous reports [S3]

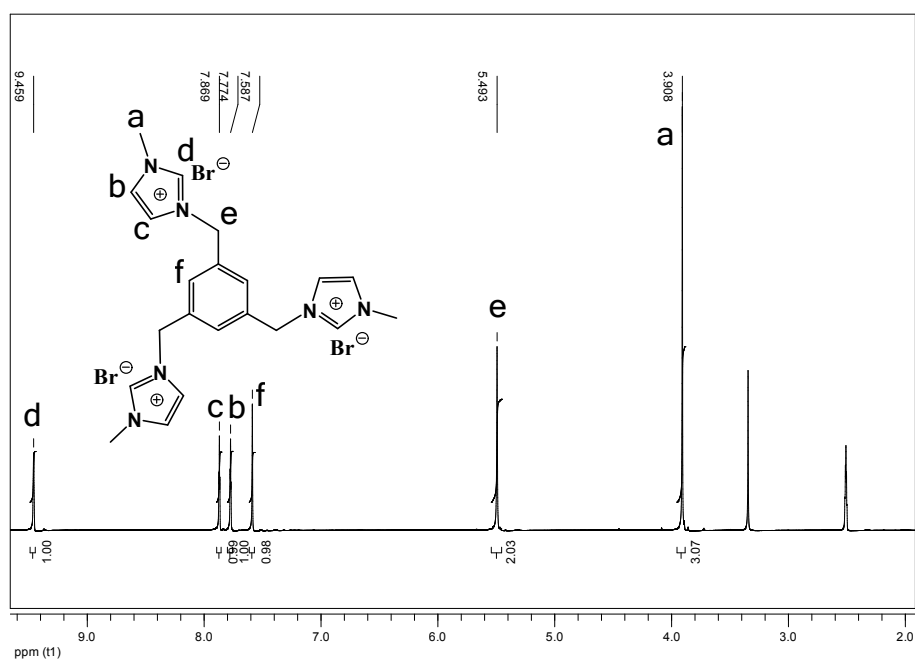


Fig. S1 ¹H NMR spectrum of 1,3,5-tris-(1-methylimidazol-3-ethyl)-benzene bromide [TMImB][Br]

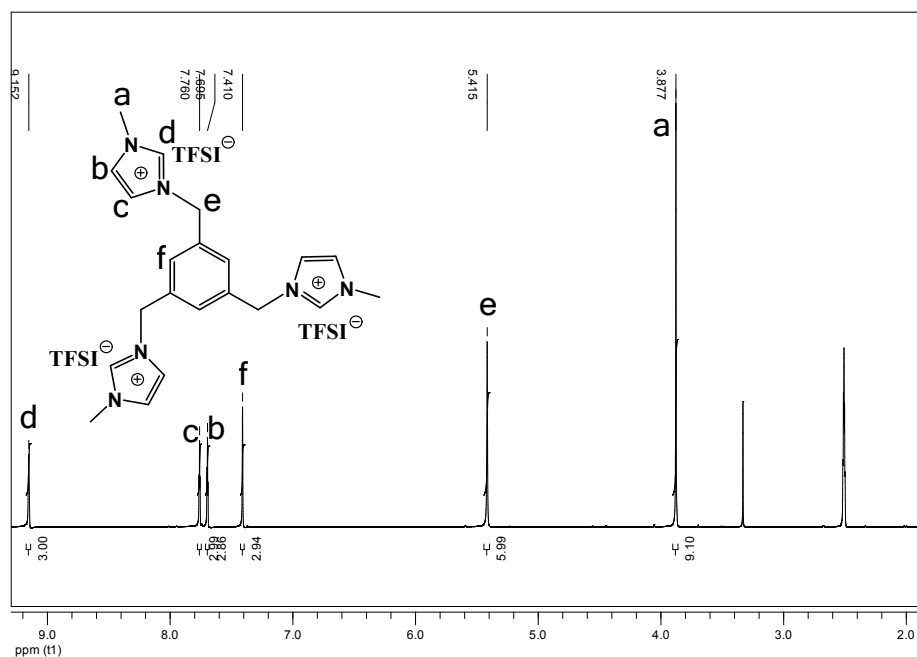


Fig. S2 ^1H NMR spectrum of 1, 3, 5-tris-(1-methylimidazol-3-ethyl)-benzene bis(trifluoromethanesulfonyl)imide [TMImB][TFSI]

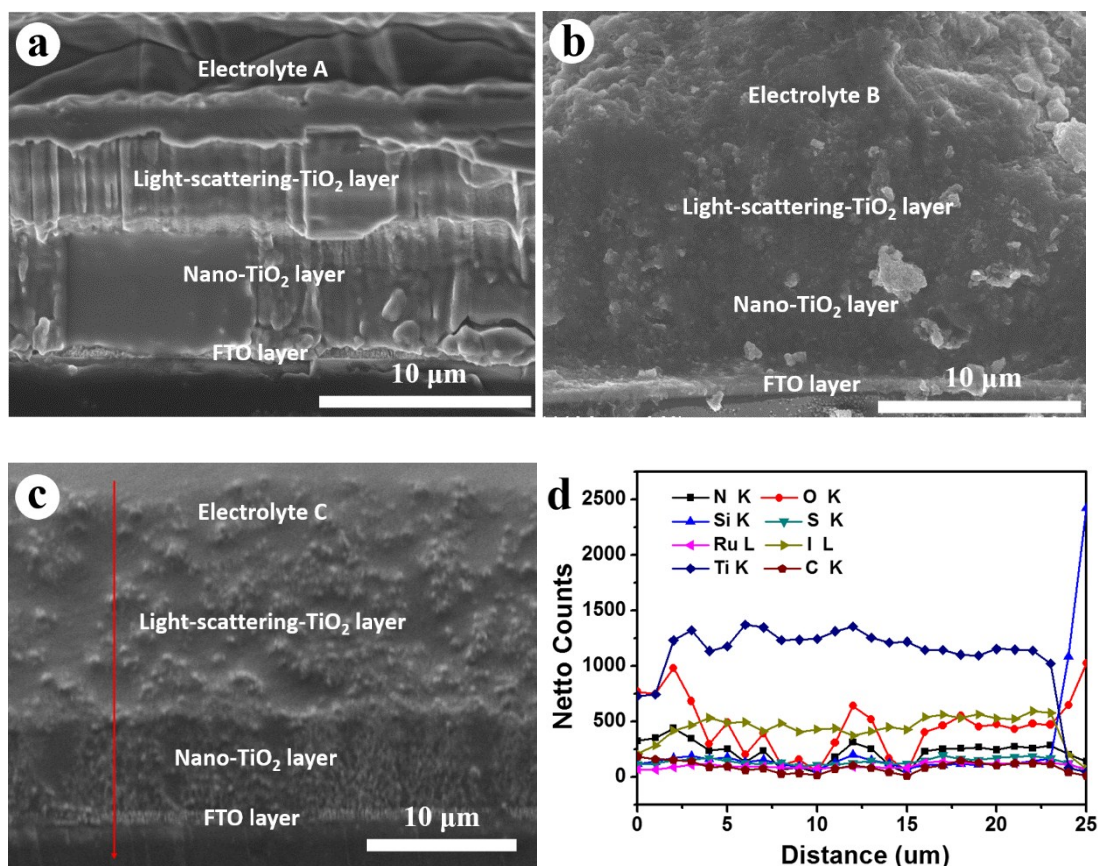


Fig. S3 (a-c) Cross-section SEM images of typical dyed-photoanodes coated with Electrolytes A-C, respectively. (d) Typical EDX line analysis of element mapping for Electrolyte C.

References

- [S1] H. Cao-Cen, J. Zhao, L. Qiu, D. Xu, Q. Li, X. Chen and F. Yan, *J. Mater. Chem.* 2012, **22**, 12842-12850.
- [S2] S. Cong, Q. Yi, Y. Wang, J. Zhao, Y. Sun and G. Zou, *J. Power Sources*, 2015, **280**, 90-96.
- [S3] J. H. Wu, Z. Lan, J. M. Lin, M. L. Huang, Y. F. Huang, L. Q. Fan, et al. *Chem. Rev.*, 2015, **115**, 2136-2173.