

Electronic Supplementary Information (ESI) for

FeSe₂ with controllable morphologies as an efficient counter electrode for dye sensitized solar cells

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Synthesis of FeSe₂ CEs

A typical synthesis process for FeSe₂ rod clusters is as follows: FeCl₃·6H₂O (1 mmol, 99%, Aladding) and Se powder (2 mmol, 99.999%, Alfa-Aesar) dissolved in deionized water (30 mL) were added to a 50 mL Teflon-lined autoclave in sequence, and then 8 mL of N₂H₄·H₂O (99%, Alfa-Aesar) was added with vigorous stirring for 10 min. Transparent conductive glass (F-doped SnO₂, FTO, 15 Ω/square) FTO was put in the autoclave and placed at an angle against the wall of the Teflon liner with the conducting side facing down. The autoclave was sealed and maintained at 140 °C for 12 h. Afterwards, the autoclave was allowed to cool down to room temperature. The synthetic process for FeSe₂ film assembled by near-spherical shaped grains was carried out under the same condition as the preparation of 3D flowerlike FeSe₂ except adding 2.0 g citric acid. To prepare Pt CEs, 5 mM H₂PtCl₆ in isopropanol was drop-cast on the 1.5×1.5 cm² FTO glass substrates, followed by heat treatment in a muffle furnace at 400 °C for 30 min and the CEs were obtained. The active area of the counter electrodes were 0.56 cm².

Fabrication of DSSCs

TiO₂ films (15 μm) containing transparent (11 μm) and scattering (4 μm) layers were prepared according to a previous report^[1]. The photoelectrodes were immersed into dye solution containing N719 (0.3 mM) at room temperature for 12 h. The dye-sensitized TiO₂ photoanode and the CE were separated by a hot-melt Surlyn film (45 μm) with an exposed area of 0.56 cm² and sealed through hot-pressing. The redox electrolyte (0.1 M LiI, 0.05 M I₂, 0.6 M

1,2-dimethyl-3-*n*-propylimidazolium iodide, and 0.5 M 4-*tert*-butylpyridine in anhydrous acetonitrile) was injected into the interspace between the photoanode and CE through the pre-drilled holes and sealed.

Measurements

X-ray diffraction (XRD) measurements were carried out with an X-ray powder diffractometer (X'Pert, Philips Inc.) with Cu K α radiation. The surface morphologies of the FeSe₂ loaded FTO glass were observed using a scanning electron microscope (SEM, FEI Quanta 200 FEG). The morphologies of the FeSe₂ samples (F_r and F_s) were observed using transmission electron microscopy (TEM, JEOL JEM-2100F). Cyclic voltammetry was performed in a three-electrode system with an acetonitrile solution containing 0.1 M LiClO₄, 10 mM LiI, and 1 mM I₂ at a scan rate of 50 mV·s⁻¹. Electrochemical impedance spectroscopy (EIS) was performed at 0 V bias by applying the ac amplitude of 10 mV in 0.1 Hz to 500 kHz frequency range with thin layer dummy cells. The geometric active area of the dummy cell was 0.56 cm². Impedance data were analyzed using commercially available Z-View software and fitted in terms of equivalent electric circuits. All the electrochemical characterizations were performed on an electrochemical workstation (Autolab 302N, Metrohm). The photovoltaic performances of the DSSCs were evaluated by a Keithley 2420 3A source meter controlled by Testpoint software under solar simulator (solar AAA simulator, oriel USA, calibrated with a standard crystalline silicon solar). A black mask with an aperture area of about 0.25 cm² was applied on the surface of DSSCs. The incident photon-to-current conversion efficiency (IPCE) spectra of DSSCs were collected with a QE/IPCE measurement kit (Newport Corporation, Irvine, CA).

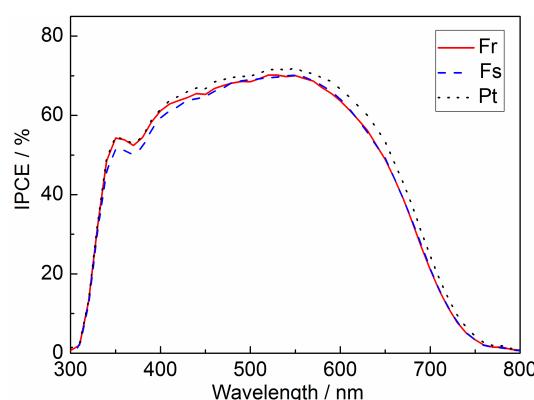


Figure S1. IPCE spectra of the corresponding DSSCs.

References

- [1] L. H. Hu, S. Y. Dai, J. Weng, S. F. Xiao, Y. F. Sui, Y. Huang, S. H. Chen, F. T. Kong, X. Pan, L. Y. Liang, K. J. Wang, *J Phys Chem B*, 2007, **111**, 358-362.