Reversible structural transformation and enhanced performance of PEDOT:PSS-based hybrid solar cells driven by light intensity

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METHODS

The hybrid solar cells were fabricated on one-side-polished, n-type Si(100) substrates (Phosphorus doped), with resistivity of 1−2 Ohm-cm and thickness of 250 ± 25 μm (Virginia Semiconductor Inc.). The substrates were ultrasonically cleaned for 10 min successively in acetone, isopropyl alcohol, Millipore water, and then dried under a nitrogen stream. The substrates were then immersed in 2% hydrofluoric acid (HF) for 10 min to remove the native oxide. After HF etching, the substrates were thoroughly cleaned in Millipore water and then the unpolished side of Si substrate was deposited with Al metal (200 nm thick) in a dual-target magnetron sputtering system (EMS575X). The substrates were then kept in an ambient air atmosphere for about 1 h for passivation of Si surface through the naturally grown SiO_x layer.

Highly conducting grade PEDOT:PSS (PH1000) was purchased from Clevios and all other chemicals were purchased from Sigma-Aldrich. The PEDOT:PSS was mixed with an optimized amount of 7 wt% EG, which is designated here as EG7-PEDOT:PSS. For spin coating, two different solutions were prepared by adding 0.25 wt% fluorosurfactant (FS-300, designated as FS) to EG7-PEDOT:PSS and pristine PEDOT:PSS. The spin-coating on planar-Si substrates was carried out at a spin rate of 6,000 rpm for 1 min and then annealed at 109±1 °C on a hot plate for 10 min in air. For solar cell property measurement, comb-type Ag metal grid electrode (50 nm thick) was sputter-deposited on the polymer layer through a shadow mask.

The solar cell properties were analysed using a solar cell characterization system capable of both *I*-*V* and EQE measurements (PV Measurements IV5 and QEX10). The *I*-

V measurements were performed under 100 mW/cm^2 illumination using a class ABA solar simulator (AM 1.5G) in air. Prior to the *I-V* measurement, a Si reference cell (PVM782 with a BK7 window) was used to calibrate the light source intensity. A metal aperture mask was used to cover and to specify the area of the device during the measurement. The calculated device area excludes the shading of Ag metal grids.

The EQE measurements were carried out under monochromatic light (in between two fingers of the top electrode), as filtered by a dual-grating monochromator from a xenon arc lamp source, coupled with a germanium photodiode. The approximate illumination area was 1×3.5 mm^2. Bias light illumination was performed with xenon arc lamp outlet placed 15 mm away from the sample and at an incident angle of 45^o with respect to the incident monochromatic light. The light-bias intensity was adjusted by increasing the voltage reading on the setup, and the intensity (power) at the sample position was measured using an energy power meter (Molectron, EPM1000e).

Reflectance spectra of the PEDOT:PSS layer on Si (without the Ag top electrodes) were collected in an ultra-violet-visible spectrometer (PerkinElmer, Lambda 35). Raman spectra were collected at room temperature with a laser wavelength of 785 nm and laser power of 50 mW in a Bruker Senterra spectrometer. The integration time was 80 s and the resolution was 3–5 cm^{-1}. The surface morphology of the PEDOT:PSS films were examined by tapping-mode atomic force microscopy (AFM) in a Digital Instruments Dimension 3100 Nanoscope IV.

Table S1. The series (R_s) and shunt (R_{sh}) resistances of the high-efficiency (Cell H) and low-efficiency cells (Cell L).

Sample	**R_s (Ω)**	**R_{sh} (Ω)**
Cell H	3.7 (3.7 ± 1)	699 (1000 ± 240)
Cell L	53.8 (55 ± 22)	146 (120 ± 50)

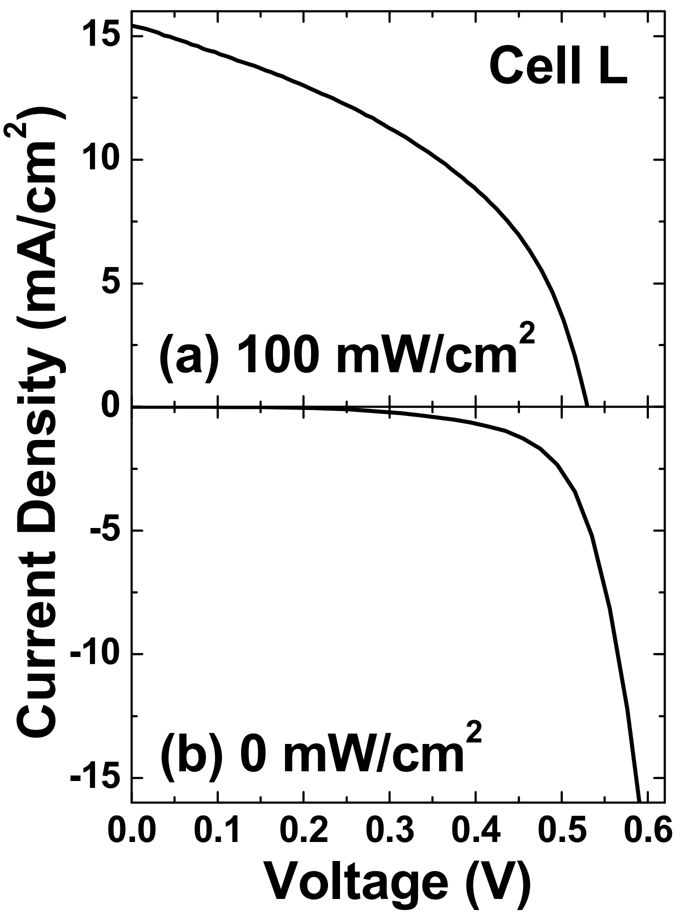

Figure S1. Current density vs voltage curve of a typical low-efficiency cell (Cell L) measured (a) under one sun (100 mW/cm^2) and (b) in the dark.

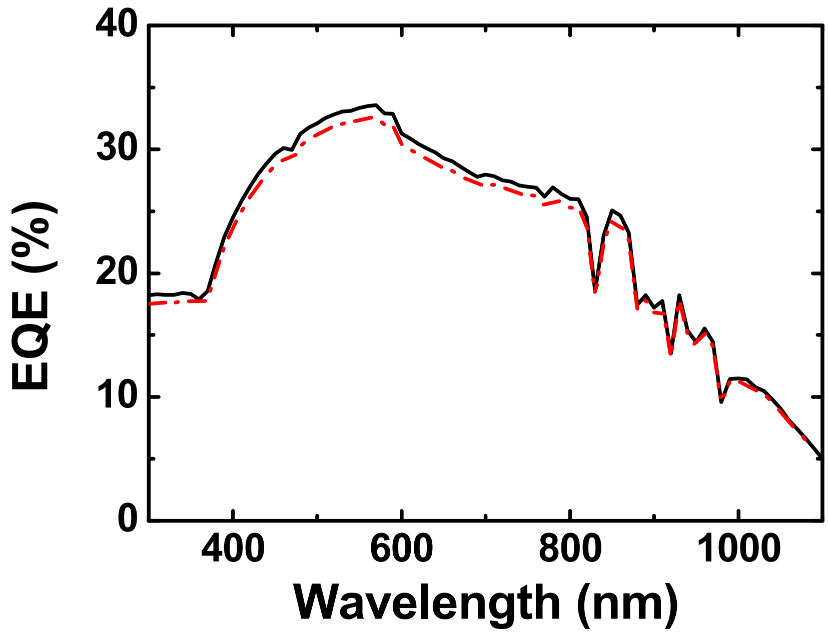

Figure S2. Typical EQE spectra of solar cell made of pristine PEDOT:PSS after exposed to light illumination of 100 mW/cm^2 for 3 h (dotted-dashed line). The spectrum (solid line) measured after the sample kept for five minutes in dark after the light illumination shows slight increase in the EQE.