Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Highly efficient inverted polymer solar cells using fullerene derivative modified TiO_2 nanorods as the buffer layer

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Experimental section

Reagent and Materials.

The ITO-coated glass substrates were provided by CSG HOLDING CO. PTB7 was purchased from 1-material Chemscitech and $PC_{71}BM$ was purchased from American Dye Source, Inc. CPTA, Chlorobenzene, 1,8-diiodoctane were purchased by Sigma-Aldrich. The Titanium tetraisopropoxide (TTIP) was obtained from J&K Scientific Ltd. Methanol, oleic acid, pyridine and chloroform were purchased from Sinopharm Chemical Reagent Co. All the chemicals were used as received without further purification.

Synthesis of TiO_2 NRs and Ligand Exchange.

Anatase TiO_2 NRs were synthesized according to the previously reported method.[1] The obtained TiO_2 NRs surface are usually attached with insulating ligands of oleic acid (OA), which prevent the aggregation of TiO_2 NRs. Original OA ligands on TiO_2 NRs surface were partially replaced by pyridine to enhance charge transport.[2, 3] The as-synthesized TiO_2 NRs were precipitated by methanol for 3 times. Then the precipitant was re-dispersed in pyridine (5ml, AR) in an ultrasonic homogenizer. The TiO_2 NRs/pyridine solution was then kept at 78^{o}C with stirring for 4h till the solution turned clear. Finally, the excess hexane was used for precipitating the TiO_2 NRs at room temperature and washing out the unabsorbed surface modifiers. The resulting precipitates were isolated by centrifugation. Then, these pyridine coated-TiO_2 NRs were re-dispersed in chloroform for device fabrication.

Device Fabrication.

PSCs were fabricated by the following procedure. The patterned ITO substrates were cleaned by ultrasonic processing in detergent, deionized water, acetone, and isopropyl alcohol. The chloroform solution of TiO_2 NRs was deposited on the ITO substrates with 1500 rpm for 40s and annealed at 150^{o}C for 15 min in the air. The thickness of bare TiO_2 film was 30 nm. Then the methanol solution of CPTA with different concentration was spin casted on TiO_2 fillms. The active layer solution of PTB7:$PC_{71}BM$ in mixed solvent of chlorobenzene/1,8-diiodoctane (97:3 vol%) at a 10:15 weight ratio was spin casted at 1500 rpm for 120s on top of the buffer layer.[4] Finally, the devices were pumped down to a ca. 1×10^{-6} mbar pressure, and a ca. 10 nm of MoO_3 and a ca. 100 nm of Al film were deposited on top of the active layer as the anode through a shadow mask to obtain the active area of 2×2 mm^2.

Characterization and Measurement.

The current density-voltage (*J-V*) characteristics of the PSCs were recorded by a Keithley 2400 source meter under exposure to an AM 1.5 Global solar simulator with an intensity of 100 mW cm^{-2}. The EQE measurements were taken by the Newport IQE-200 Measurement System, which was equipped with a monochromator, a Xe lamp, a lock-in amplifier, and a current-voltage preamplifier. The surface height images of the samples were obtained by atomic force microscope (AFM). AFM was operated using a Veeco dimension V atomic microscope in tapping mode at room temperature. The water contact angle measurements were performed by dropping deionized water using Contact Angle System OCA-20.

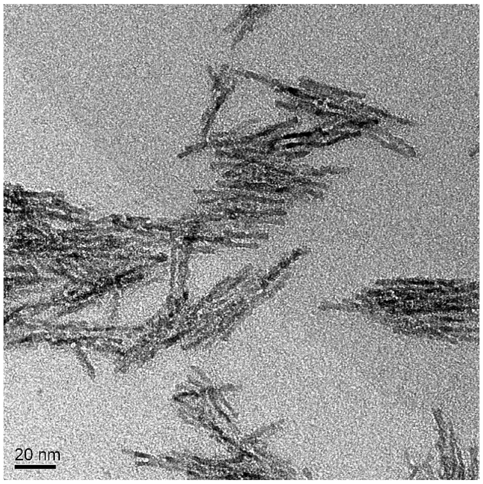

Figure S1. TEM image of TiO_2 nanorods.

Table S1. Specific devices parameters based on TiO_2 NRs modified with the different concentrations of CPTA as the buffer layer in PTB7:$PC_{71}BM$ blends.

Concentration (mg/ml)	V_{oc} [V]	J_{sc} [mA cm^{-2}]	FF [%]	η [%]	R_s Ω cm^2	R_{sh} Ω cm^2
0	0.758	14.69	69.6	7.75	5.24	1021
0.5	0.757	15.73	73.5	8.74	3.88	1567
0.7	0.757	15.49	72.2	8.47	4.52	1336
1	0.750	15.48	71.4	8.29	5.60	1148

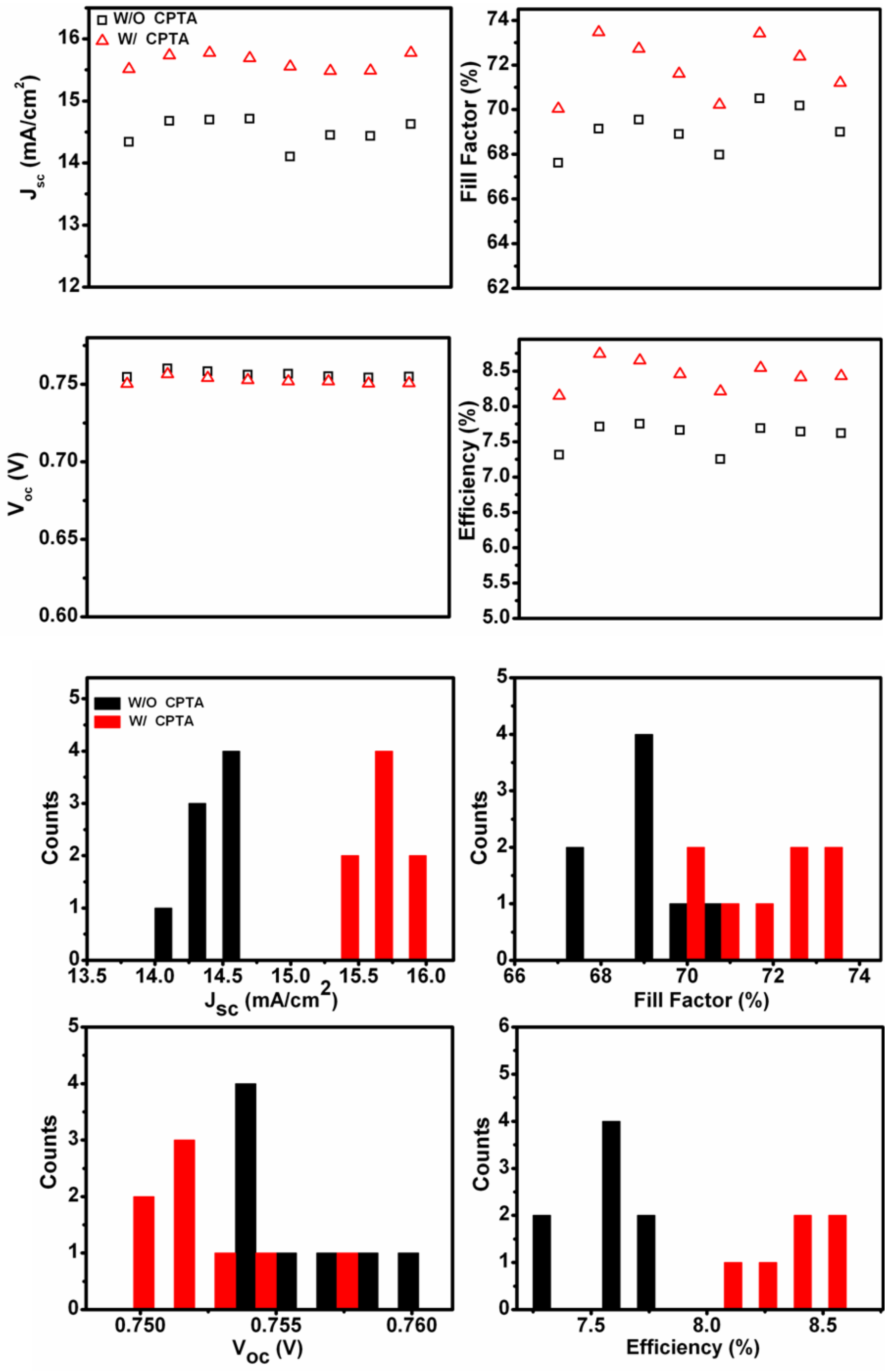

Figure S2. The device parameter distribution maps using bare TiO_2 or CPTA-modified TiO_2 as the buffer layer in PSCs.

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