Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

Replacing the metal oxide layer with a polymer surface modifier for high-performance inverted polymer solar cells

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Experimental Section

Materials and instruments: For device fabrication, a poly[[4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-b:4,5-b']dithiophene-2,6-diyl][3-fluoro-2-[(2-ethylhexyl)-carbonyl]thieno-[3,4-b]thiophenediyl]] (PTB7) was purchased from 1-Material and poly(3-hexylthiophene) (P3HT, M_W=50,000 g mol-1, ~95% regioregularity), [6,6]-phenyl-C60 butyric acid methyl ester ($PC_{60}BM$, Rieke Metal inc.), and [6,6]-phenyl-C_{70} butyric acid methyl ester ($PC_{70}BM$), were purchased from Rieke Metal Inc.. Polyethylenimine, 80% ethoxylated (PEIE, M_w=70,000 g mol^{-1}, 35~40% in H_2O) was purchased from Aldrich. Reflectance spectra were measured on a Varian Cary 5000 spectrophotometer. The atomic force microscopy (AFM) images (1.5 μm × 1.5 μm) were obtained using a VeecoAFM microscope in a tapping mode. Contact angles were measured using DSA100 (KRUSS, Germany). Thickness of active layer was measured using Surface Profiler (KLA_Tencor).

Solar cells fabrication and characterization: Indium tin oxide (ITO) substrates were sequentially cleaned with detergent, water, acetone, and isopropanol. For bilayer devices, zinc oxide (ZnO) precursor solution prepared using sol-gel method and then this solution was spin-coated onto an ITO substrate and annealed at 110 °C for 10 min.[1] The PEIE solution (35~45 wt% in H_2O) diluted further in 2-methoxyethanol (0.4 wt%) was spin-coated on top of ZnO film and annealed at 100°C for 10 min. For bilayer devices, The PTB7 (1 wt%) or P3HT solution (2 wt%) was spin-cast on top of ZnO or ZnO/PEIE films in nitrogen filled glove box. For bulk-heterojunction (BHJ) devices, ZnO and PEIE films were deposited using same methods with bilayer devices. 1,2-dichlorobenzene (DCB) solution with 1,8-diiodooctane (DIO) (DCB:DIO = 97:3 (vol%)) containing PTB7 (1 wt%) and $PC_{70}BM$ (1.5 wt%) was spin-cast at 800 rpm on top of different electron selective layer (ESL). The DCB solution containing P3HT (2 wt%) and $PC_{60}BM$ (2 wt%) was also spin-cast at 700 rpm on top of different ESL. The thicknesses of the PTB7:$PC_{70}BM$ and P3HT:$PC_{60}BM$ BHJ films were about 150 nm and 200 nm, respectively. Subsequently, the device was pumped down under vacuum (< 10^{-6} Torr), and the p-type MoO_3 (5 nm) and Au (100 nm) were sequentially deposited. The area of the Au electrode defines an active area of the device as 13.0 mm^2. Measurements were carried out inside a glove box by using a high quality optical fiber to guide the light from a solar simulator equipped with a Keithley 2635A source measurement unit. A mask (13.0 mm^2) made of a thin metal was attached to each cell for the photovoltaic characteristics measurements under AM 1.5G illumination at 100 mW cm^{-2}.

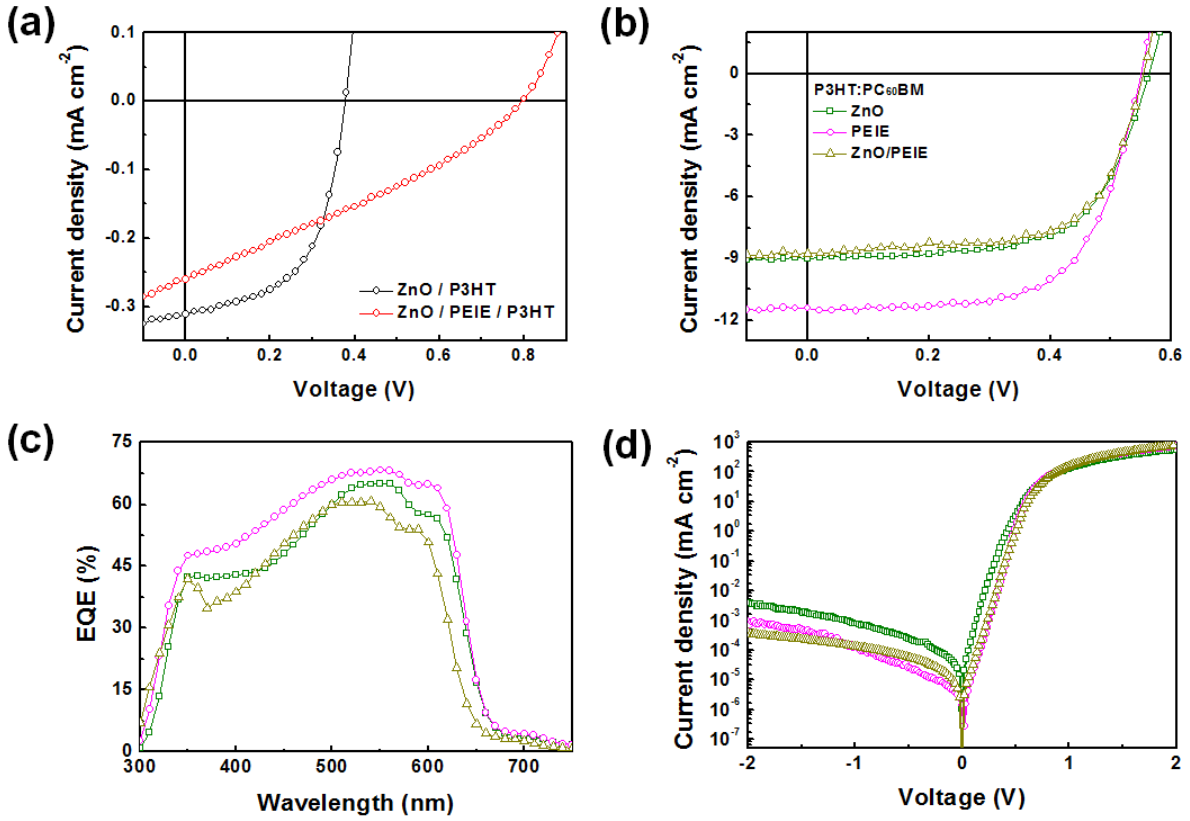

Fig. S1 Comparison of *J-V* characteristics in (a) P3HT/ZnO-based bilayer and (b) P3HT:$PC_{60}BM$-based BHJ devices with different ESL layer, and (c) corresponding external quantum efficiency (EQE) curves of BHJ devices. (d) Dark *J-V* characteristics of BHJ devices with ZnO or PEIE layer.

Table S1. Characteristics of P3HT/ZnO-based bilayer and P3HT:$PC_{60}BM$-based BHJ devices with different ESL.

Device configuration	J_{sc} [mA cm^{-2}]	V_{oc} [V]	*FF*	PCE [%]	J_{sc}(Calc.) [mA cm^{-2}]
ITO/ZnO/P3HT/MoO_3/Au	0.31	0.38	0.55	0.06	-
ITO/ZnO/PEIE/P3HT/MoO_3/Au	0.26	0.80	0.30	0.06	-
ITO/ZnO/P3HT:$PC_{60}BM$/MoO_3/Au	9.03	0.56	0.63	3.21	9.25
ITO/PEIE/P3HT:$PC_{60}BM$/MoO_3/Au	11.4	0.55	0.64	4.04	10.4
ITO/ZnO/PEIE/P3HT:$PC_{60}BM$/MoO_3/Au	8.76	0.55	0.64	3.12	8.17

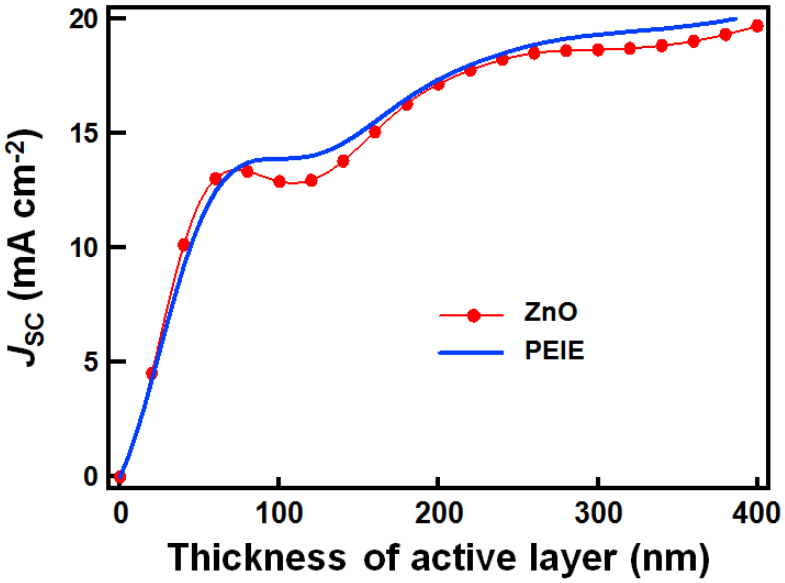

Fig. S2 Estimated J_{SC} value of the devices with ZnO and PEIE layer as a function of active layer thickness. Since the effect of ultrathin PEIE layer (below 10 nm) on light absorption was negligible, we performed optical modeling using the device structures with and without ZnO layer.

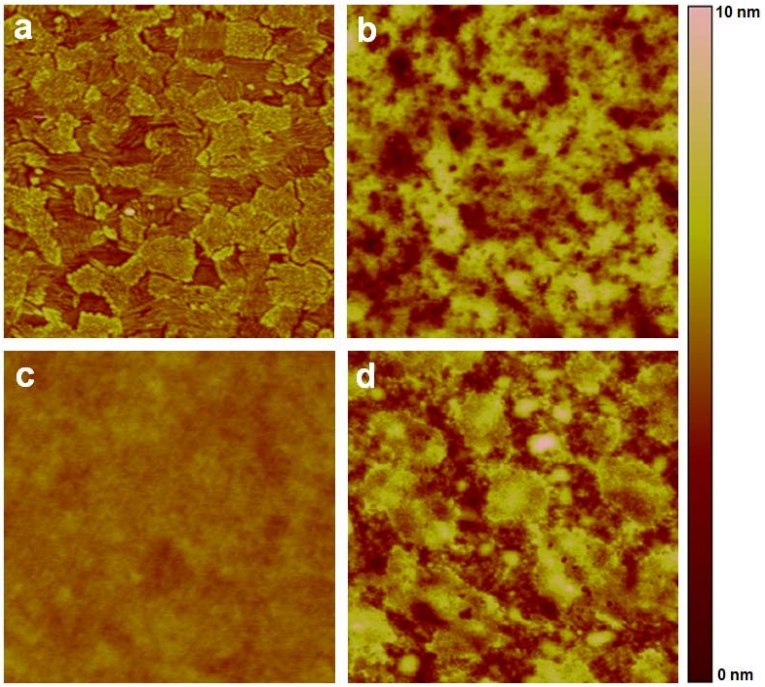

Fig. S3 Tapping-mode AFM topography images of (a) bare ITO, (b) ZnO, (c) PEIE, and (d) ZnO/PEIE films spin-coated on ITO substrate. AFM image size is 1.5 μm x 1.5 μm.

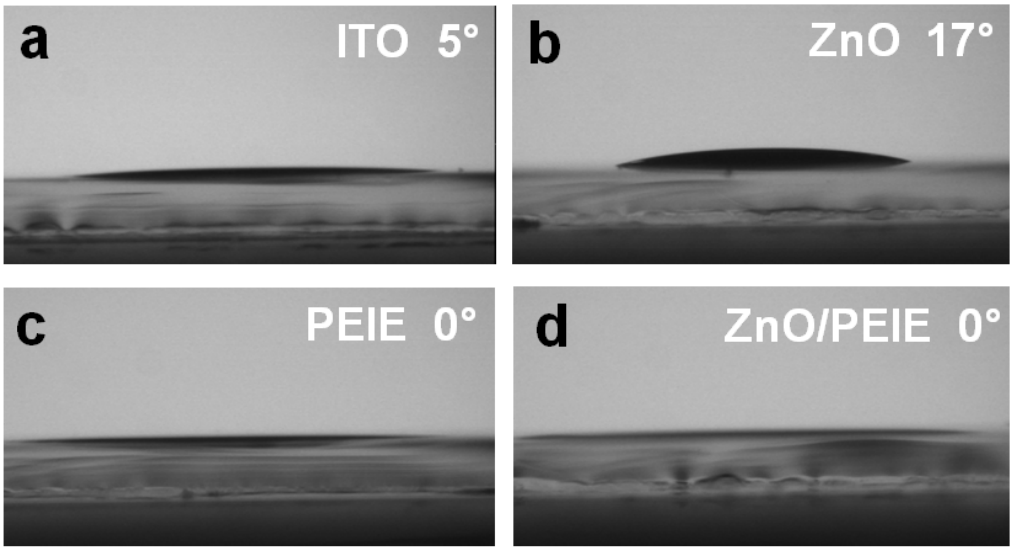

Fig. S4 Contact angle measurements of (a) UV-treated ITO, (b) ZnO, (c) PEIE, and (d) ZnO/PEIE films to mixed solvent of dichlorobenzene and 1,8-diiodooctane.

References

1 W. J. E. Beek, L. H. Slooff, M. M. Wienk, J. M. Kroon and R. A. J. Janssen, *Adv. Funct. Mater.*, 2005, **15**, 1703.