Supplementary Information

Adenine-based Polymer Modifying Zinc Oxide for Efficient Inverted Organic Solar Cells

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Materials: Zinc acetate (ZnAc), potassium hydroxide (KOH) were purchased from J&K. 2,2,2-Trifluoroethanol (99.8%) and 1-chloronaphthalene (85%) were purchased from Acros. 1,8-diiodoctane (98%) and chlorobenzene (99.8%) were purchased from Sigma Aldrich. PTB7 was purchased from 1-Material, and $PC_{71}BM$ was purchased from Nano-C. PM6 was obtained from Solamer, Inc. Y6 was purchased from eflexpv.

Instrumentation: The AFM measurements were conducted on a DMFASTSCAN2-SYS (Bruker, USA) in tapping mode with a 5μm scanner at 1Hz speed. Film thickness was determined by the surface profiler manufactured by Bruker (model DEKTAK-XT) and samples were made on pre-cleaned glass substrates. XPS measurements were carried out by ESCALAB 250 (Thermo Fisher Scientific USA), equipped with monochromatic Al Kalph 150 W X-ray source. The SKP scans were conducted on SKP5050 (KP Technology Ltd.). The samples for SKP measurements were prepared on ITO substrates. The contact angle was tested by multi-functional tensiometer (Krùss DSA30). The samples for contact angle measurements were prepared on glass substrates. ^{1}H NMR spectra were recorded on a Bruker Avance III 400 (400 MHz) spectrometer in DMSO-d6. Gel permeation chromatography (GPC) was performed using a Shimadzu GPC system (using low dispersity polystyrene as standard) equipped with 10 μm mixed columns in series and in line with a 20 A refractive index detector. DMAc (with 0.3g/L LiBr and 0.5g/L BHT) was used as eluent at a flow rate of 1 mL/min.

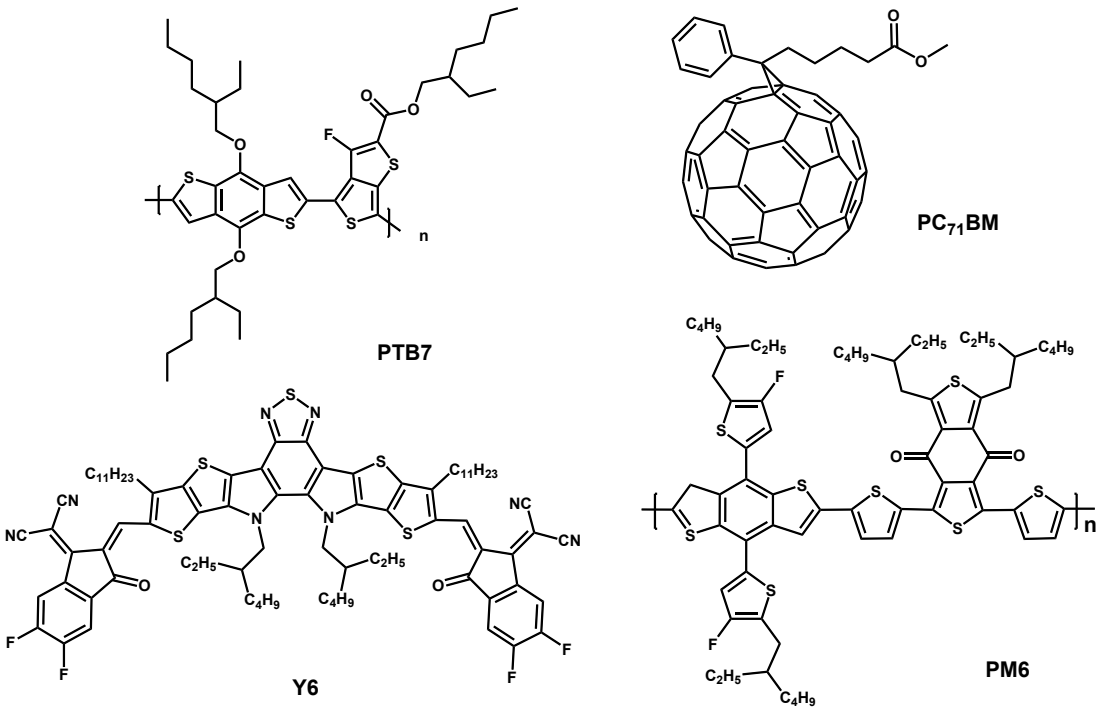

Figure S1. Chemical structures of photoactive layer materials.

Table S1. The photovoltaic parameters of devices based ZnO interlayers with or without post treatment (the average values and standard deviations are calculated from 5 devices).

ETL	Post treatment	V_{OC} (V)	J_{SC} (mA/cm^2)	*FF* (%)	PCE (%)
ZnO	no	0.74±0.01	14.91±0.17	64.16±1.77	7.03±0.17
	150 ℃ annealing	0.74±0.01	14.69±0.21	64.83±1.01	7.01±0.11

Table S2. Photovoltaic parameters of PTB7: $PC_{71}BM$ devices with normal geometry structure using ZnO nanoparticle interlayers (the average values and standard deviations are calculated from 5 devices).

ETL	V_{OC} (V)	J_{SC} (mA/cm^2)	*FF* (%)	PCE (%)
ZnO	0.71±0.01	14.69±0.29	57.98±2.51	6.05±0.43

Table S3. The performance of PTB7:$PC_{71}BM$ based devices containing ZnO nanoparticle interlayers modified with different **PA** weight ratio (the average values are calculated from 15 devices and the optimal PCEs are listed in brackets).

Interlayers	**PA** (wt%)	V_{OC} (V)	J_{SC} (mA/cm^2)	Calculated J_{SC} (mA/cm^2)	*FF* (%)	PCE (%)
ZnO	0	0.73±0.01	14.79±0.19	14.60	64.73±1.65	7.01±0.14(7.29)
ZnO:PA	5	0.74±0.01	15.72±0.01	15.17	67.11±0.01	7.75±0.01(8.06)
	15	0.75±0.01	16.06±0.19	15.32	70.10±0.83	8.42±0.16(8.70)
	25	0.76±0.01	16.07±0.08	15.39	71.79±0.81	8.73±0.09(8.88)
	30	0.76±0.01	15.87±0.12	15.30	69.47±0.79	8.37±0.14(8.68)

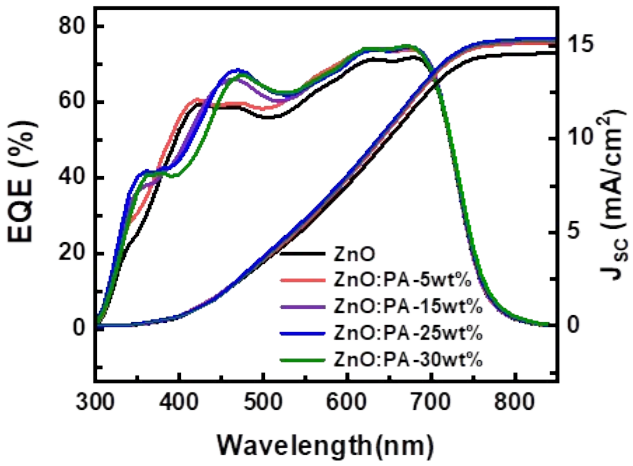

Figure S2. EQE spectra of PTB7:$PC_{71}BM$ based devices containing ZnO nanoparticle interlayers modified with different **PA** weight ratio.

Table S4. Stability measurements of devices based on PTB7: $PC_{71}BM$ with the pristine or **PA**-modified ZnO nanoparticle interlayers (the average values and standard deviations are calculated over 5 devices).

Interlayers	Time (h)	V_{OC} (V)	J_{SC} (mA/cm^2)	*FF* (%)	PCE (%)	Stability (%)
ZnO	0	0.73±0.01	14.64±0.41	66.58±2.55	7.21±0.23	100
	24	0.73±0.01	14.56±0.67	62.43±3.04	6.69±0.26	93
	48	0.73±0.02	13.66±0.76	61.01±4.14	6.09±0.47	85
	72	0.73±0.02	13.37±1.15	61.00±6.39	5.95±0.44	83
	120	0.73±0.01	12.78±0.44	58.32±3.44	5.47±0.22	76
	240	0.72±0.01	12.65±0.24	56.24±5.75	5.11±0.55	71
	360	0.69±0.01	12.86±0.59	55.46±5.75	4.94±0.57	69
	480	0.67±0.02	12.50±0.50	45.27±5.84	3.79±0.59	53
ZnO:PA (25%)	0	0.75±0.00	15.96±0.08	71.38±0.90	8.57±0.17	100
	24	0.75±0.00	15.64±0.12	71.57±1.35	8.50±0.27	99
	48	0.75±0.00	15.53±0.17	70.96±1.83	8.37±0.16	98
	72	0.75±0.01	15.55±0.20	70.60±1.25	8.27±0.11	96
	120	0.75±0.01	15.26±0.14	71.09±1.25	8.17±0.13	95

240	0.76±0.00	15.13±0.29	69.91±1.13	8.21±0.19	96
360	0.75±0.00	15.32±0.14	69.21±1.36	7.99±0.18	93
480	0.75±0.00	15.17±0.17	69.75±0.94	7.99±0.16	93

Table S5. Photovoltaic parameters of PM6: Y6 devices in **Figure 2C** (the average values and standard deviations are calculated from 15 devices).

Interlayers	**PA** (wt%)	V_{OC} (V)	J_{SC} (mA/cm^2)	Calculated J_{SC} (mA/cm^2)	*FF* (%)	PCE (%)
ZnO	0	0.83±0.01	23.68±0.50	23.01	70.40±1.58	13.83±0.32(14.31)
ZnO:PA	25	0.85±0.01	25.56±0.32	24.43	73.85±1.05	16.04±0.11(16.22)

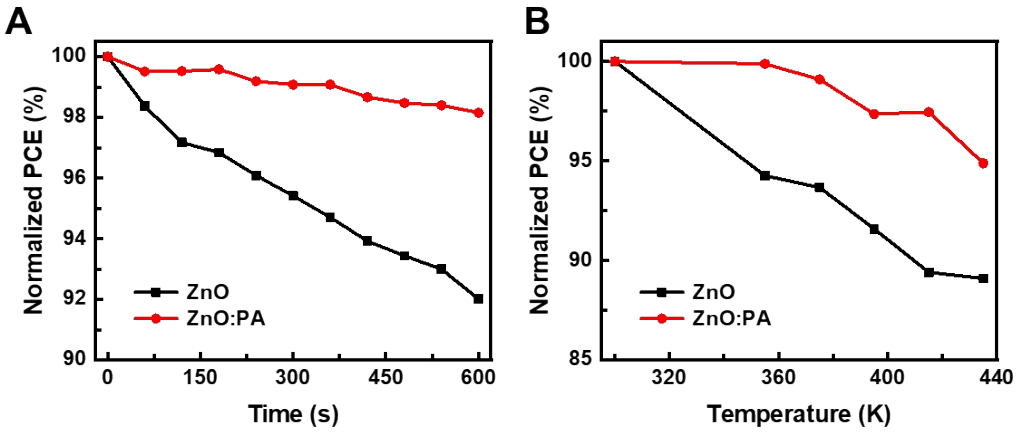

Figure S3. (A) The stabilized power output of the PM6:Y6 based devices containing pristine ZnO nanoparticle films or ZnO nanoparticle films with 25% PA modification; (B) thermal stability measurements of PM6:Y6 devices at the temperature range 300 K-435 K.

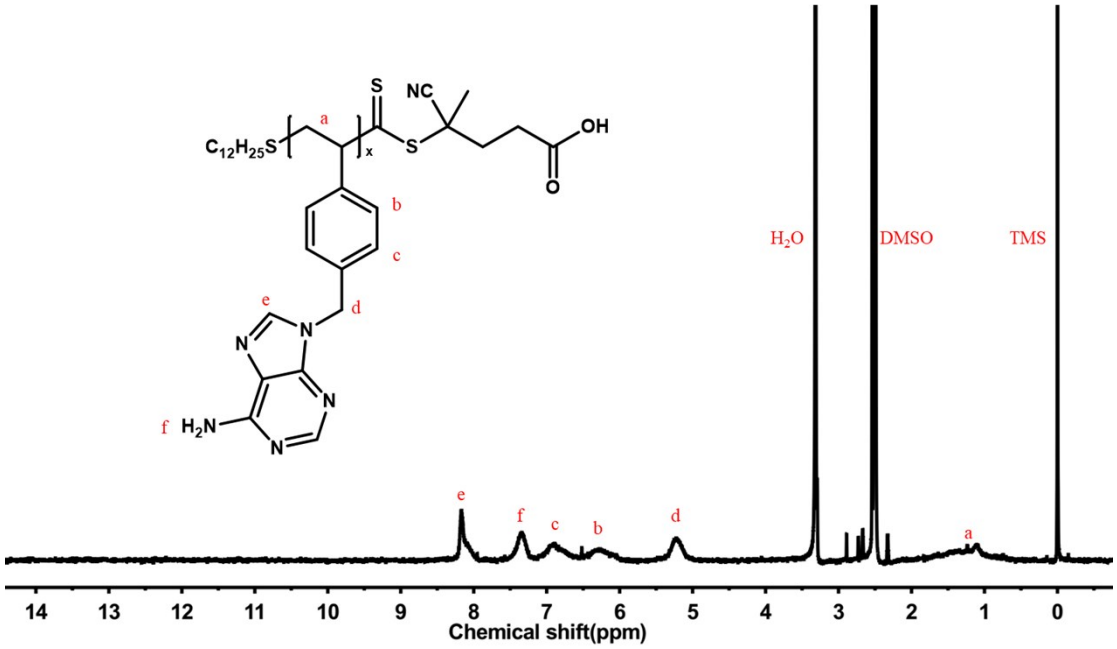

Figure S4. ^{1}H NMR spectrum of PA dispersed in DMSO-d_6.

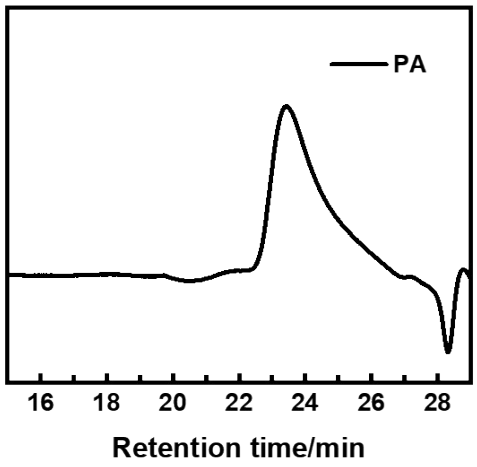

Figure S5. The GPC traces of PA (Mn = 8.1kDa, Mw/Mn = 1.10).