Supporting Information

Poly(3-hexylthiophene)/zinc phthalocyanine composites for advanced interface engineering of 10.03%-efficiency $CsPbBr_3$ perovskite solar cells

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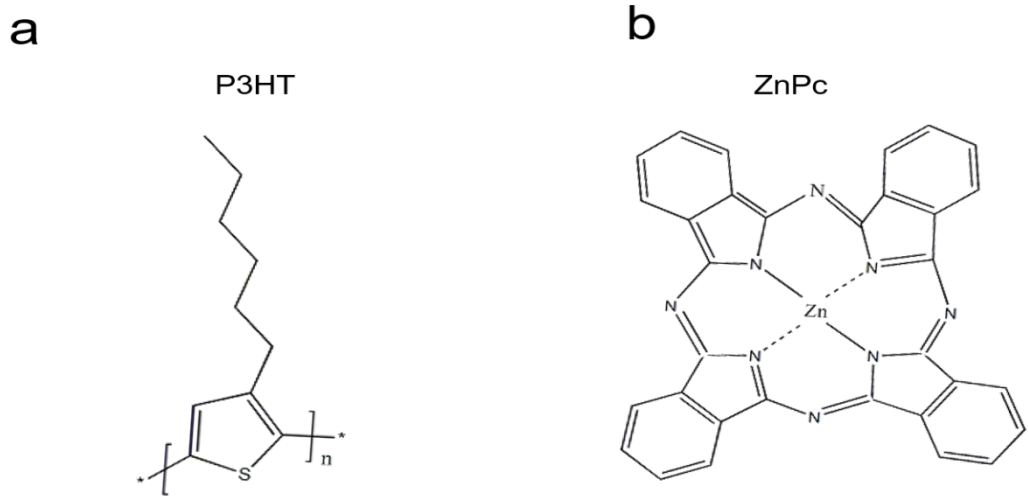

Fig. S1. Chemical structures of (a) P3HT and (b) ZnPc.

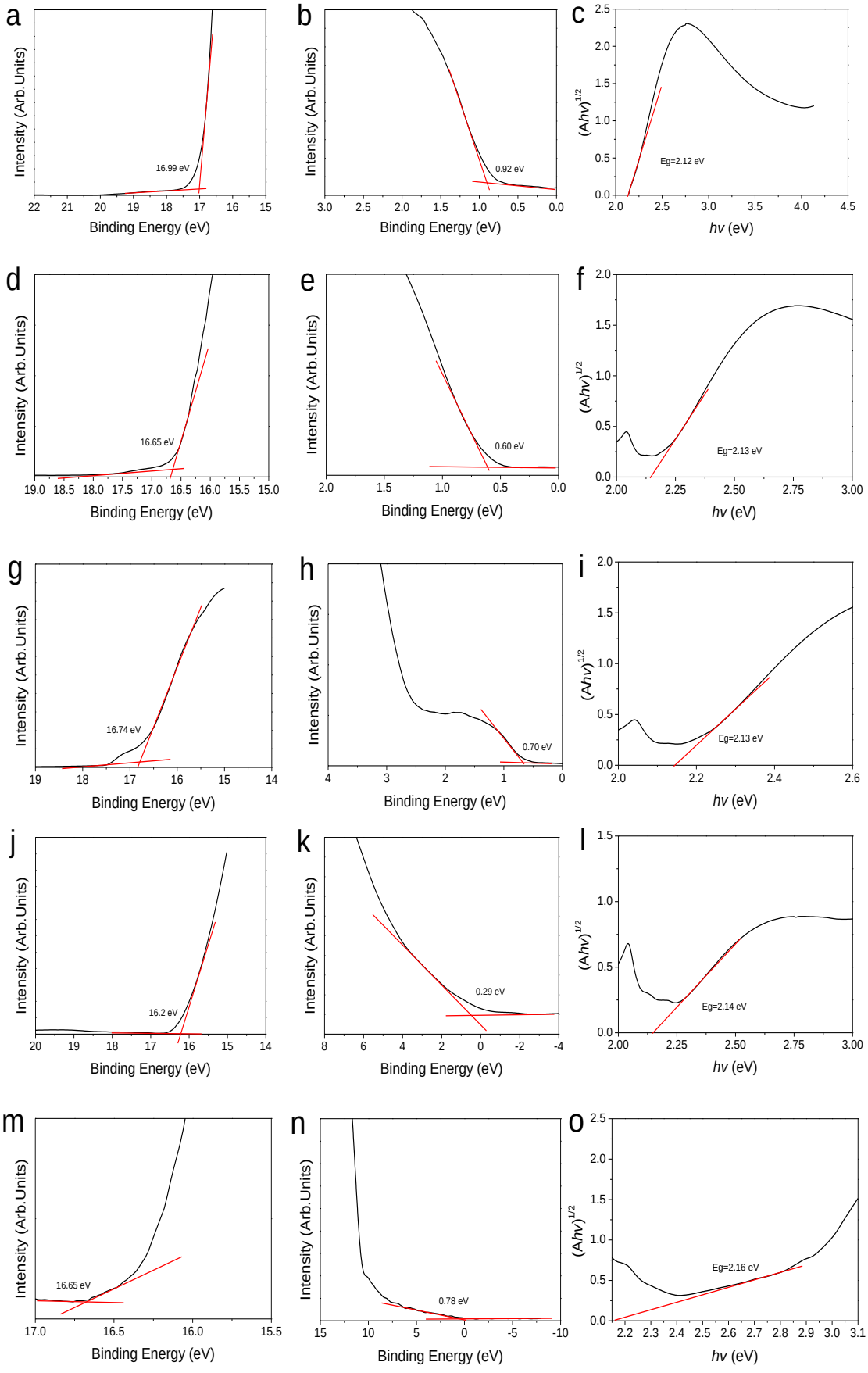

Fig. S2. UPS of (a) and (b) P3HT, (d) and (e) P2Z1, (g) and (h) P1Z1, (j) and (k)

P1Z2, and (m) and (n) ZnPc. The curves of $(Ahv)^{1/2}$ as a function of hv for (c) P3HT, (f) P2Z1, (i) P1Z1, (l) P1Z2 and (o) ZnPc.

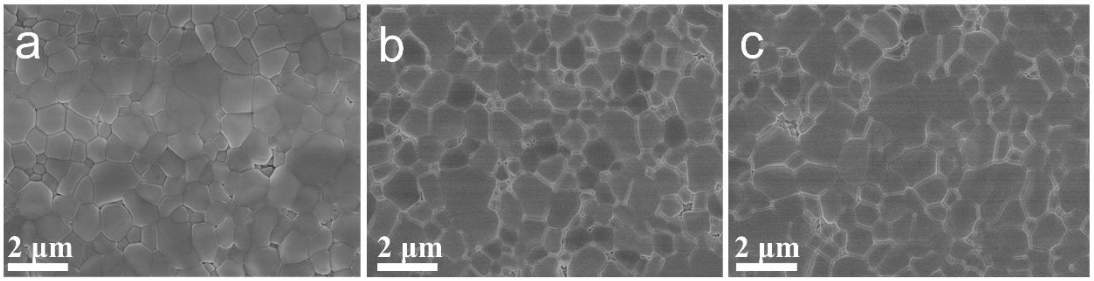

Fig. S3. Top-view SEM images of $CsPbBr_3$ after (a) 200 °C annealed, (b) CB treated, and (c) 200 °C annealed after CB treated.

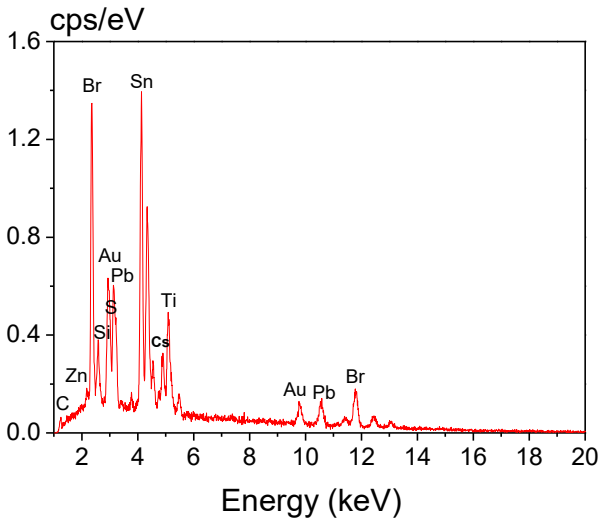

Fig. S4. EDS of P1Z1 deposited on $CsPbBr_3$ film.

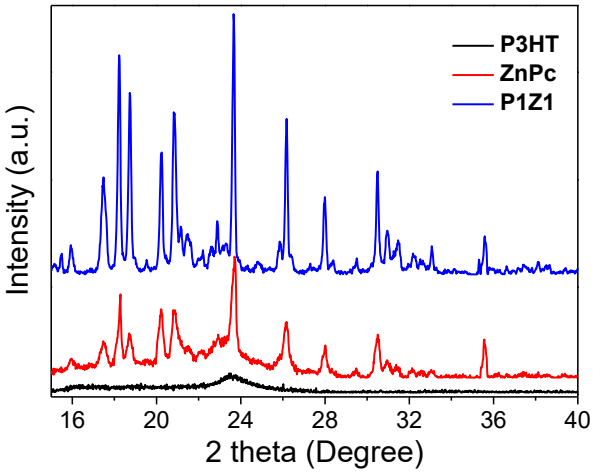

Fig. S5. The XRD patterns of ZnPc, P3HT and P1Z1 powder.

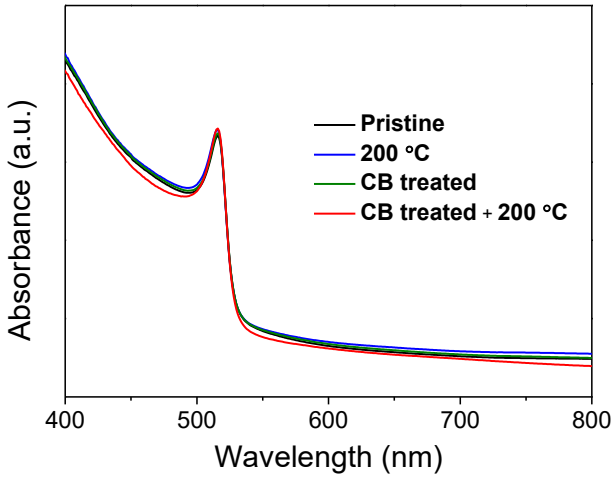

Fig. S6. UV-vis absorption spectra of pristine $CsPbBr_3$, and $CsPbBr_3$ after 200 °C annealed, CB treated, and 200 °C annealed after CB treated.

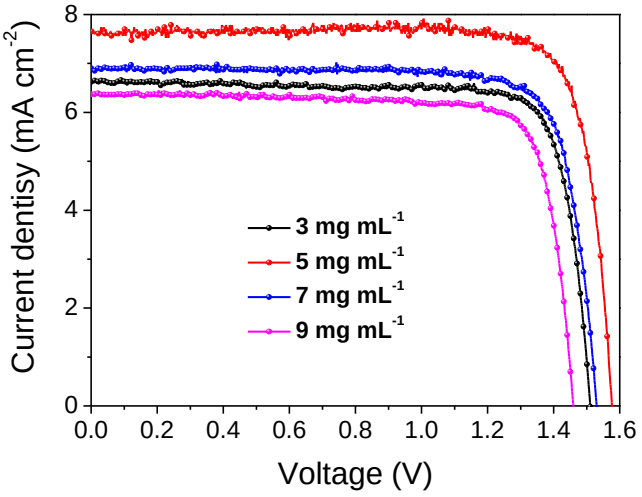

Fig. S7. Photocurrent–voltage (*J–V*) curves under air mass 1.5 global (AM1.5G, 100 mW cm $^{-2}$) for $CsPbBr_3$ PSCs based on P1Z1 HTM with different concentrations.

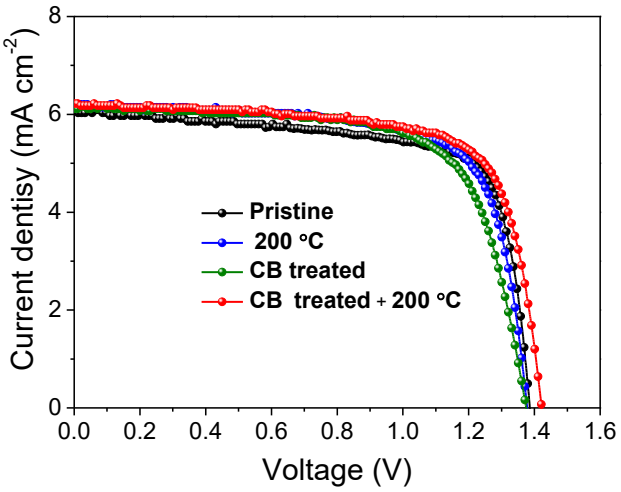

Fig. S8. Photocurrent–voltage (*J*–*V*) curves of device based on pristine $CsPbBr_3$, and $CsPbBr_3$ after 200 °C annealed, CB treated, and 200 °C annealed after CB treated.

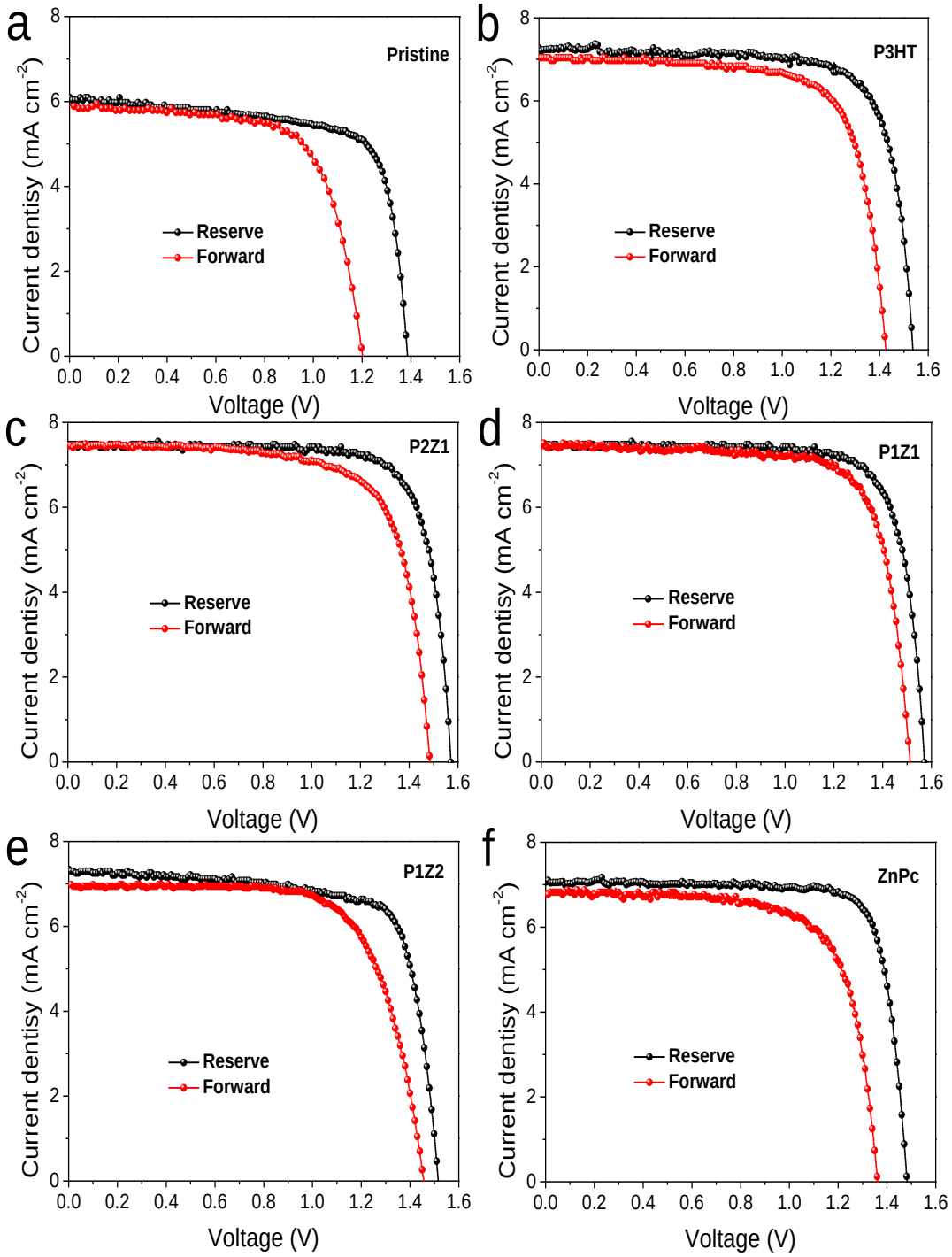

Fig. S9. Photocurrent–voltage (*J–V*) curves of $CsPbBr_3$ PSCs with and without HTMs under forward and reverse scan directions.

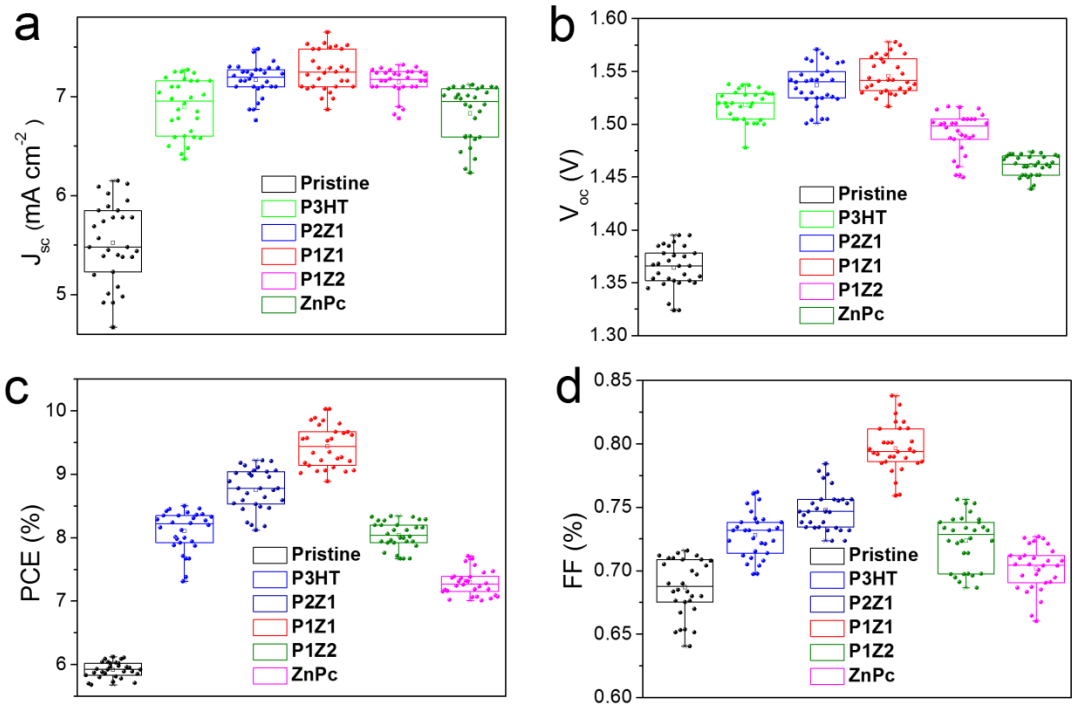

Fig. S10. Statistical distribution of the photovoltaic parameters of $CsPbBr_3$ PSCs with and without HTMs. (a) Distribution of J_{sc}. (b) Distribution of V_{oc}. (c) Distribution of ~~*FF*~~ and (d) Distribution of ~~PCE~~.

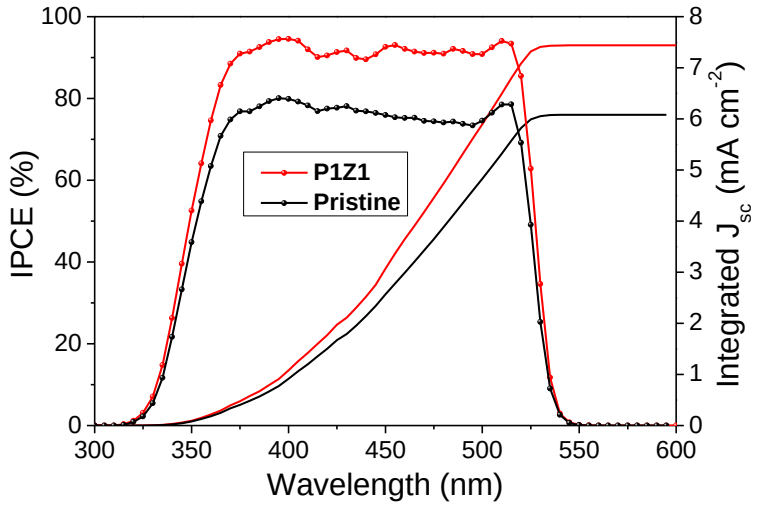

Fig. S11. IPCE spectra of HTM-free and P1Z1 HTM based $CsPbBr_3$ PSCs.

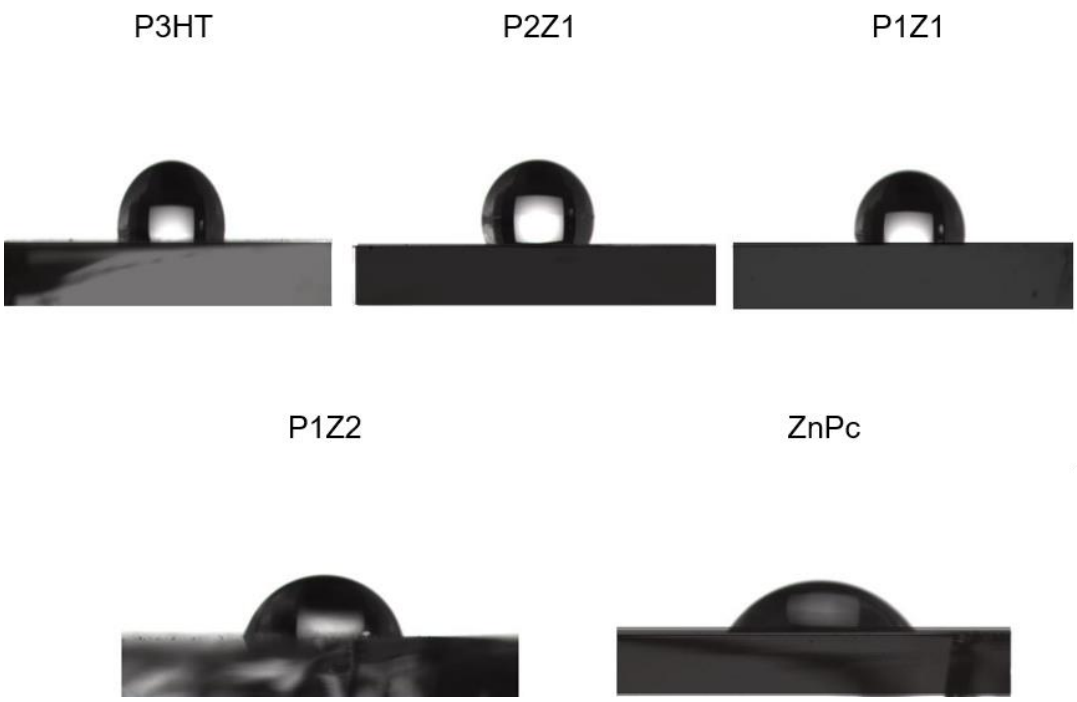

Fig. S12. Contact angle of 99.7°, 113.1°, 101.2°, 74.0° and 52.3° for P3HT, P2Z1, P1Z1, P1Z2 and ZnPc, respectively.

Table S1. The HOMO, LUMO energy levels and bandgaps of differetn HTMs.

HTM	P3HT	P2Z1	P1Z1	P1Z2	ZnPc
LUMO (eV)	-3.01	-3.02	-3.03	-3.15	-3.17
HOMO (eV)	-5.13	-5.15	-5.16	-5.29	-5.33
E_g (eV)	2.12	2.13	2.13	2.14	2.16

Table S2. TRPL decay parameters of excitonic transitions for $CsPbBr_3$ PSCs with and without HTMs..

HTMs	HTM-free	P3HT	P2Z1	P1Z1	P1Z2	ZnPc
τ_1 (ns)	0.32	0.18	0.07	0.05	0.08	0.15
f_1 (%)	43.60	62.20	83.72	88.84	88.07	39.54
τ_2 (ns)	2.04	1.3913	0.97	0.89	1.37	1.74
f_2 (%)	56.40	37.80	16.28	11.16	11.93	60.46
τ_{ave} (ns)	0.60	0.27	0.07	0.06	0.09	0.34

τ_{ave} ~~(ns)~~ = $(f_1\tau_1^2 + f_2\tau_2^2)/ (f_1\tau_1 + f_2\tau_2)$

Table S3. Photovoltaic parameters of $CsPbBr_3$ PSCs based on P1Z1 HTM with different concentrations.

P1Z1 HTM	J_{sc} (mA cm^{-2})	V_{oc} (V)	*FF* (%)	PCE (%)
3 mg mL^{-1}	6.62	1.511	82.07	8.21
5 mg mL^{-1}	7.652	1.578	83.06	10.03
7 mg mL^{-1}	6.67	1.497	81.12	8.57
9 mg mL^{-1}	6.37	1.46	81.29	7.56

Table S4. Photovoltaic parameters of device based on pristine $CsPbBr_3$, and $CsPbBr_3$ after 200 °C annealed, CB treated, and 200 °C annealed after CB treated.

$CsPbBr_3$	J_{sc} (mA cm^{-2})	V_{oc} (V)	*FF* (%)	PCE (%)
Pristine	6.15	1.390	71.59	6.12
200 °C	6.2	1.378	72.05	6.16
CB treated	6.12	1.376	69.77	5.87
CB treated + 200 °C	6.22	1.423	72.09	6.38

Table S5. EIS parameters of $CsPbBr_3$ PSCs with and without HTMs.

HTMs	R_s (Ω cm^2)	R_{rec} (Ω cm^2)	CPE (nF cm^{-2})
HTM-free	4.60	21.03	118.18
P3HT	3.46	78.77	50.67
P1Z1	3.43	106.07	32.49
ZnPc	4.55	30.46	56.19