

Supporting Information

Efficient Carbon-based CsPbI₂Br Perovskite Solar Cells using Bifunctional Polymer Modification

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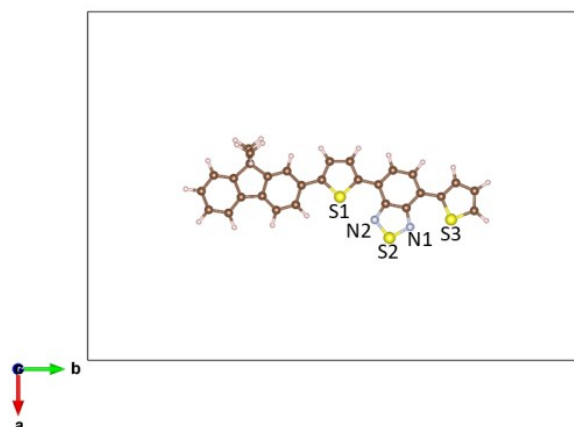


Figure S1. The label of atom in the monomers of PTDTBT molecule.

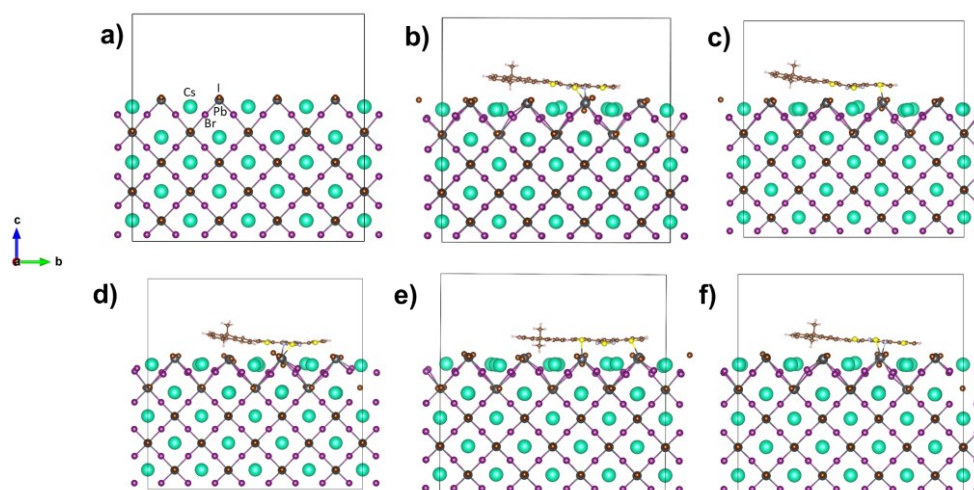


Figure S2. Atomic structure of optimized CsPbI₂Br (001) surface with adsorbed PTDTBT. **a)** CsPbI₂Br (100), **b)** N₁-Pb-S₂, **c)** N₂-Pb-S₂, **d)** 2S₁-Pb, **e)** S₂-Pb-N₁, **f)** S₃-Pb.

Table S1. Adsorption energy of different atoms interacting with perovskite.

	E(eV)	ΔE(eV)
PTDTBT	-365.08014	-
CsPbI ₂ Br	-856.79954	-
N1-Pb-S2	-1221.4575	0.42218
N2-Pb-S2	-1221.3694	0.51028
2S1-Pb	-1221.1487	0.73098
S2-Pb-N1	-1212.9055	8.97418
S3-Pb	-1212.5540	9.32568

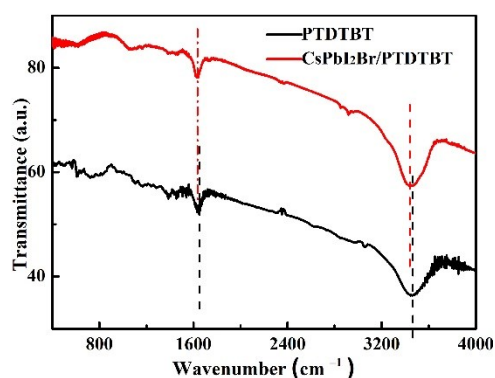


Figure S3. Fourier transform infrared (FTIR) spectra of PTDTBT and CsPbI₂Br/PTDTBT, respectively.

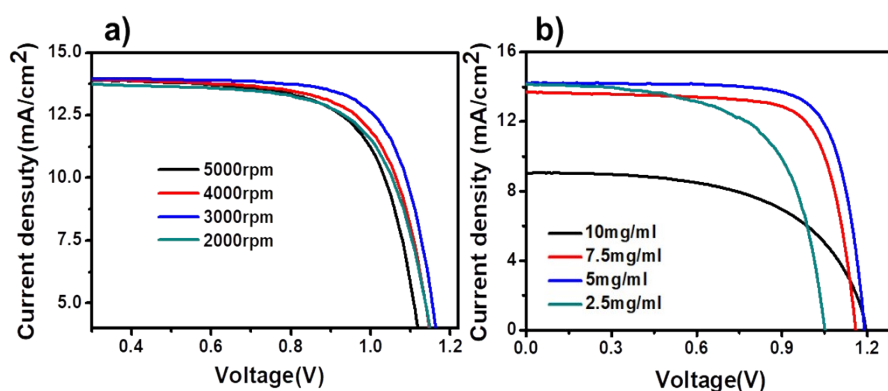


Figure S4. J - V curves of devices with PTDTBT processed by **a)** different spin coating speed and **b)** different concentration.

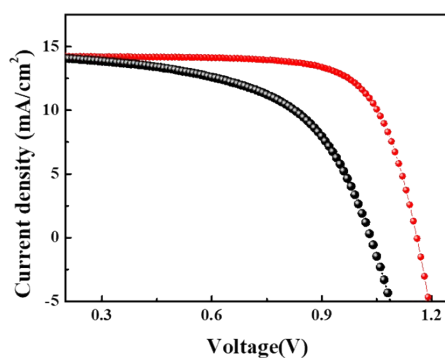


Figure S5. J - V curve of the device obtained at a concentration of 5mg/ml PFDTBT (the scan directions of red line and black line are reverse scan (RS) and forward scan (FS), respectively.)

Table S2 Device performance parameters with PTDTBT processed by different concentrations of HTM.

Concentration(mg/ml)	J_{sc} (mA/cm ²)	V_{oc} (V)	FF (%)	PCE (%)
2.5	14.3	1.10	70.21	11.04
5	14.2	1.19	75.91	12.83
7.5	13.9	1.18	75.82	12.43
10	9.11	1.20	53.10	5.82

Table S3. Device performance parameters with PTDTBT processed by different spin coating speed.

Spin coating(rpm)	J_{sc} (mA/cm ²)	V_{oc} (V)	FF (%)	PCE (%)
2000	14.0	1.15	74.67	12.05
3000	14.2	1.17	76.01	12.63
4000	14.3	1.16	75.26	12.41
5000	14.3	1.12	72.11	11.55

Table S4. Fitting parameters of TRPL decay spectra based on CsPbI₂Br -film and CsPbI₂Br /PTDTBT-film.

Films	τ_1 (ns)	τ_2 (ns)	τ_{ave} (ns)
CsPbI ₂ Br -film	4.5550	9.2752	2.04
CsPbI ₂ Br /PTDTBT-film	18.3664	31.3710	32.83

Table S5. Device performance parameters.

Device	J_{sc} (mA/cm ²)	V_{oc} (V)	FF (%)	PCE (%)
Control	14.2±0.21	1.09± 0.31	67.1±3.9	10.81±0.87
PFDTBTDT	14.2±0.15	1.18±0.14	78.2±1.6	12.83±0.41

Table S6. The specific performance parameters corresponding to the J - V curve measured in the reverse and forward scanning directions.

Spin coating(rpm)	J_{sc} (mA/cm ²)	V_{oc} (V)	FF (%)	PCE (%)
Reverse scanning	14.0	1.07	62.12	9.31
Forward scanning	14.0	1.19	76.01	12.67