

Figure S1:  $^1\text{H}$  NMR spectra in  $\text{DMSO}-d_6$  of (a) pure 3-TPT and 3-TPT mixed with  $\text{CsPbI}_2\text{Br}$ , and (b) pure 4-TPT and 4-TPT mixed with  $\text{CsPbI}_2\text{Br}$ .

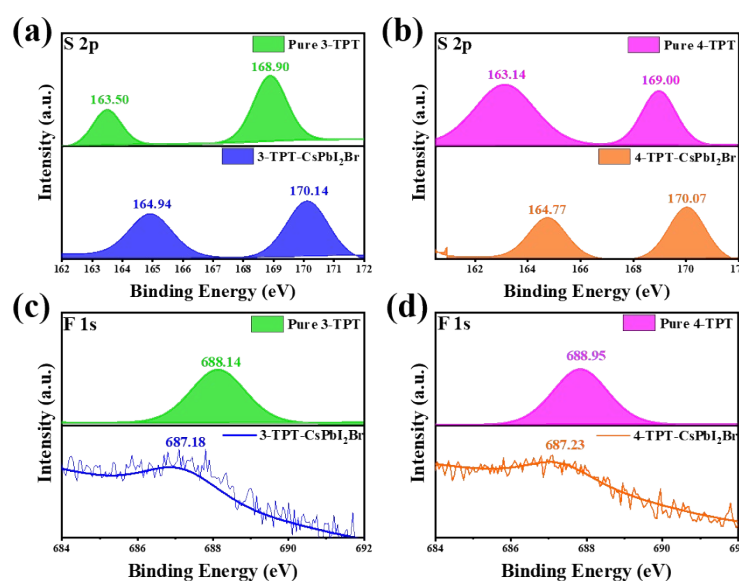


Figure S2: XPS  $\text{S } 2p$  spectra of (a) pure 3-TPT and 3-TPT- $\text{CsPbI}_2\text{Br}$ , and (b) pure 4-TPT and  $\text{CsPbI}_2\text{Br}$ ; XPS  $\text{F } 1s$  spectra of (c) pure 3-TPT and 3-TPT- $\text{CsPbI}_2\text{Br}$ , and (d) pure 4-TPT and 4-TPT- $\text{CsPbI}_2\text{Br}$ .

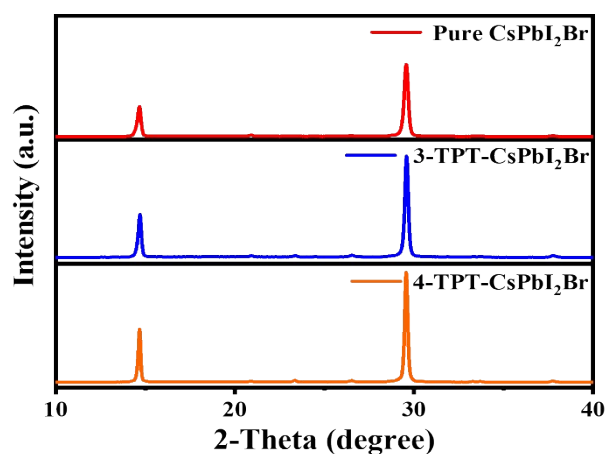


Figure S3: XRD patterns for pure  $\text{CsPbI}_2\text{Br}$ , 3-TPT- $\text{CsPbI}_2\text{Br}$ , and 4-TPT- $\text{CsPbI}_2\text{Br}$ .

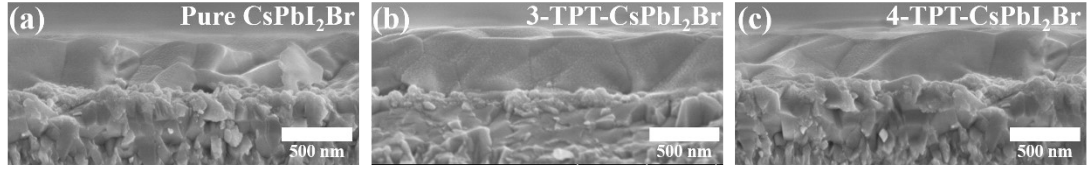


Figure S4: Cross-sectional SEM images of (a) CsPbI<sub>2</sub>Br, (b) 3-TPT-CsPbI<sub>2</sub>Br, and (c) 4-TPT-CsPbI<sub>2</sub>Br.

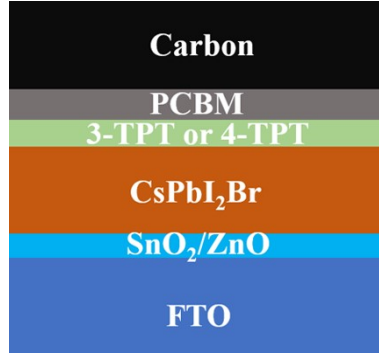


Figure S5: Schematic representation of the structure of carbon-based CsPbI<sub>2</sub>Br devices (FTO/SnO<sub>2</sub>/ZnO/CsPbI<sub>2</sub>Br/ 3-TPT or 4-TPT/PCBM/ carbon) for SCLC.

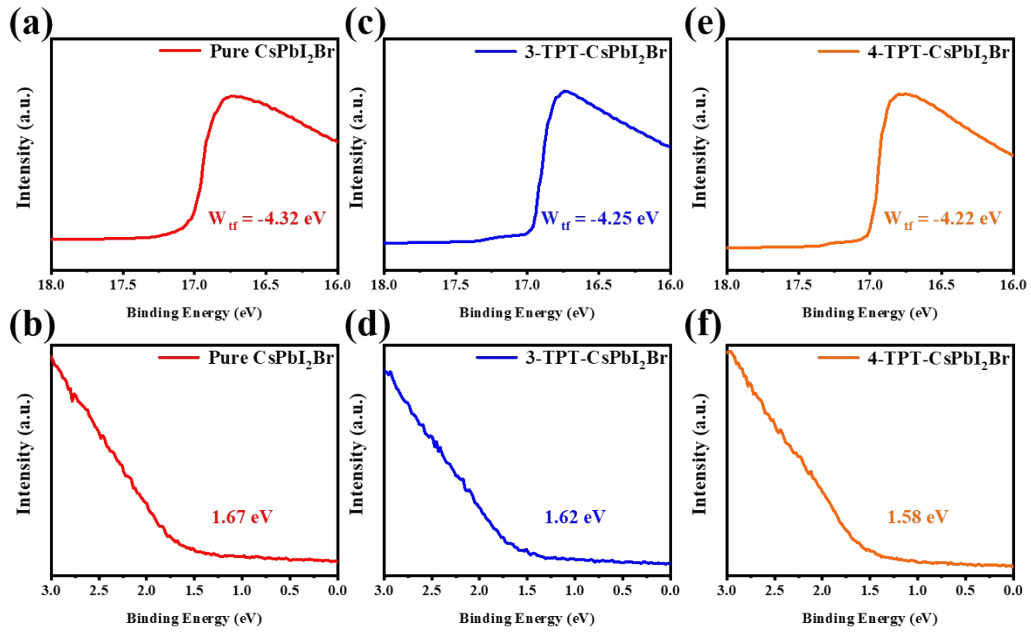


Figure S6: Ultraviolet photoelectron spectroscopic (UPS) analysis of (a) pure CsPbI<sub>2</sub>Br, (b) 3-TPT-CsPbI<sub>2</sub>Br, and (c) 4-TPT-CsPbI<sub>2</sub>Br.

Table S1. The optical properties of CsPbI<sub>2</sub>Br, 3-TPT-CsPbI<sub>2</sub>Br and 4-TPT-CsPbI<sub>2</sub>Br by UPS characterization.

| Sample                       | $E_{\text{cut-off}}$ (eV) | $E_V - E_F$ (eV) | $E_F$ (eV) | $E_V$ (eV) | $E_C$ (eV) | $E_g$ (eV) |
|------------------------------|---------------------------|------------------|------------|------------|------------|------------|
| Pure CsPbI <sub>2</sub> Br   | 16.90                     | 1.67             | 4.32       | 5.99       | 4.07       | 1.92       |
| 3-TPT- CsPbI <sub>2</sub> Br | 16.97                     | 1.62             | 4.25       | 5.87       | 3.95       | 1.92       |
| 4-TPT- CsPbI <sub>2</sub> Br | 17.02                     | 1.58             | 4.20       | 5.78       | 3.86       | 1.92       |

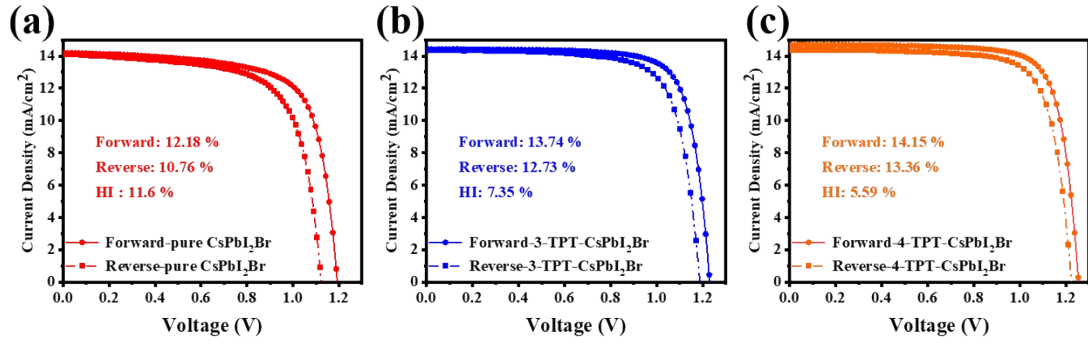


Figure S7: The J-V curves for pure CsPbI<sub>2</sub>Br, 3-TPT-CsPbI<sub>2</sub>Br, and 4-TPT-CsPbI<sub>2</sub>Br devices in both forward and reverse scans.

Table S2. Performance parameters of pure CsPbI<sub>2</sub>Br, 3-TPT-CsPbI<sub>2</sub>Br, and 4-TPT-CsPbI<sub>2</sub>Br devices in both forward and reverse scans, derived from J-V curves.

| Sample                              | V <sub>oc</sub> (V) | J <sub>sc</sub> (mA/cm <sup>2</sup> ) | Fill factor | PCE (%) | HI (%) |
|-------------------------------------|---------------------|---------------------------------------|-------------|---------|--------|
| Forward-Pure CsPbI <sub>2</sub> Br  | 1.19                | 14.19                                 | 72.14       | 12.18   | 11.66  |
| Reverse-Pure CsPbI <sub>2</sub> Br  | 1.12                | 14.10                                 | 68.12       | 10.76   |        |
| Forward-3-TPT-CsPbI <sub>2</sub> Br | 1.23                | 14.42                                 | 77.47       | 13.74   | 7.35   |
| Reverse-3-TPT-CsPbI <sub>2</sub> Br | 1.19                | 14.37                                 | 74.48       | 12.73   |        |
| Forward-4-TPT-CsPbI <sub>2</sub> Br | 1.25                | 14.47                                 | 78.22       | 14.15   | 5.59   |
| Reverse-4-TPT-CsPbI <sub>2</sub> Br | 1.22                | 14.39                                 | 76.25       | 13.39   |        |

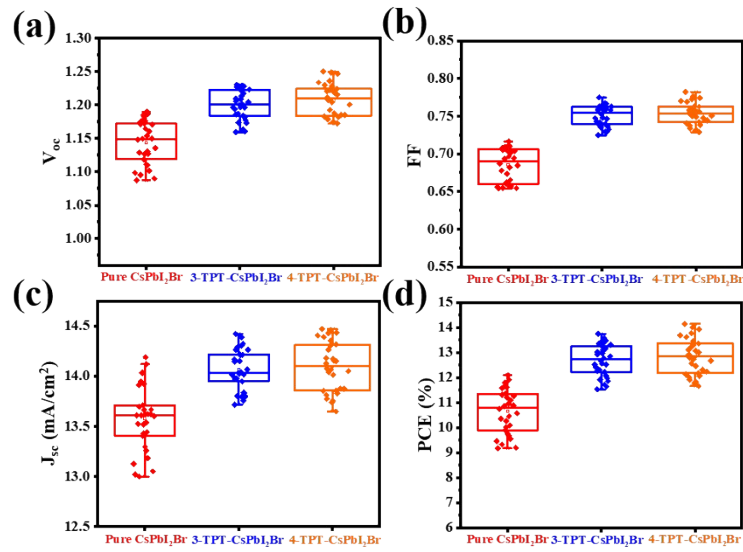


Figure S8: Boxplot distributions for 30 solar cell devices based on pure CsPbI<sub>2</sub>Br, 3-TPT-CsPbI<sub>2</sub>Br, and 4-TPT- CsPbI<sub>2</sub>Br, illustrating (a) V<sub>oc</sub>, (b) FF, (c) J<sub>sc</sub>, and (d) PCE.