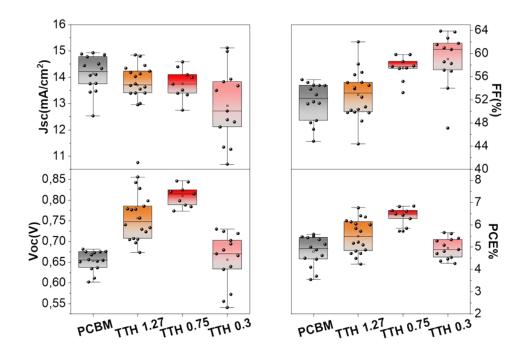
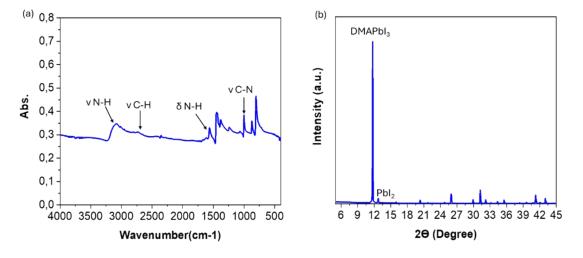
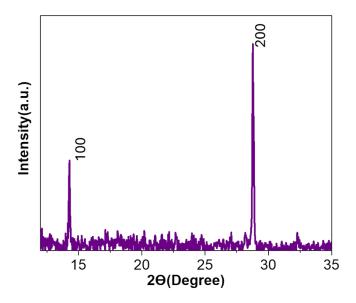
Supporting Information



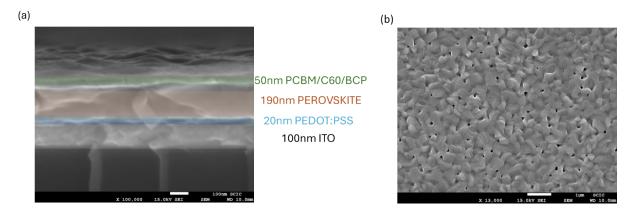
Supplementary Figure S1 I Statistical photovoltaic parameters obtained for PCBM and TTH at different concentrations 1,27mg/ml; 0,75mg/ml and 0,3mg/ml in CB.



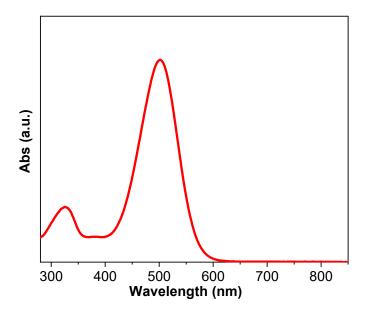
Supplementary Figure S2 I The ATR-FTIR (a) and XRD patterns (b) of synthesizing DMAPbI₃ powder precursor.



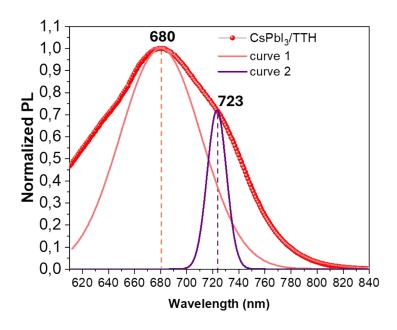
Supplementary Figure 3 I XRD patterns of CsPbI₃ powder precursor.



Supplementary Figure 4 I The cross-section and surface SEM images of the stack cell (a) and CsPbI₃ perovskite film (b).



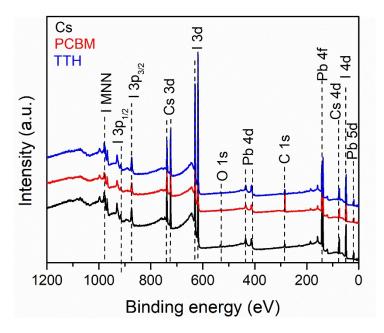
Supplementary Figure 5 I Absorption spectra of TTH molecule.



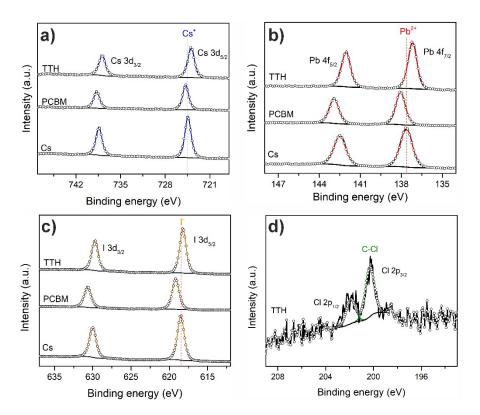
Supplementary Figure 6 I Deconvolution of photoluminescence from CsPbI₃/TTH sample.

Supplementary Table 1 I Elemental quantification of CsPbI₃ (Cs), CsPbI₃ + PCBM (PCBM) and CsPbI₃ + TTH (TTH) perovskites by XPS.

| Sample Identifier | Atomic concentration [%] | | | | | | |
|----------------------|--------------------------|------|-------|-------|-------|------|------|
| | C | 0 | Ι | Pb | Cs | Cl | N |
| Cs | 24.98 | 4.96 | 42.61 | 10.70 | 16.75 | - | - |
| Cs+PCBM | 56.66 | 3.25 | 23.88 | 6.06 | 8.05 | - | 2.10 |
| Cs + TTH | 28.00 | 2.82 | 41.32 | 9.99 | 13.05 | 1.58 | 3.25 |



Supplementary Figure 7 I XPS survey spectra of CsPbI₃ (Cs), CsPbI₃ + PCBM (PCBM) and CsPbI₃ + TTH (TTH) perovskites.



Supplementary Figure 8 I XPS high-resolution spectra of CsPbI₃ (Cs), CsPbI₃ + PCBM (PCBM) and CsPbI₃ + TTH (TTH) samples, a) Cs 3d, b) Pb 4f, c) I 3d and d) Cl 2p.

Calculated Adsorption Energies (ΔE_{ads})

Supplementary Table 2 I Adsorption Energies for one ETL molecule (PCBM and TTH) with and without D3 dispersion interactions for the half and full coverage interfaces.

| Coverage | System | $\Delta E_{ads} \le D3$ | ΔE_{ads} w/o D3 |
|----------|--------------|-------------------------|-------------------------|
| Half | CsPbI3@1TTH | -0.80 | 0.00 |
| пан | CsPbI3@1PCBM | -1.49 | -0.14 |
| Full | CsPbI3@2TTH | -0.84 | -0.01 |
| | CsPbI3@2PCBM | -1.81 | -0.13 |

As we can see, by moving from the half to full coverage the ΔE ads per molecule is increasing indicating a stabilizing effect due to the molecules packing. This effect is more pronounced in the PCBM case.