Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.
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Supplementary Information

Simultaneous realization of bulk and interface regulation based on 2,4-Diamino-6,7-diisopropylpteridine phosphate for efficient and stable inverted perovskite solar cells

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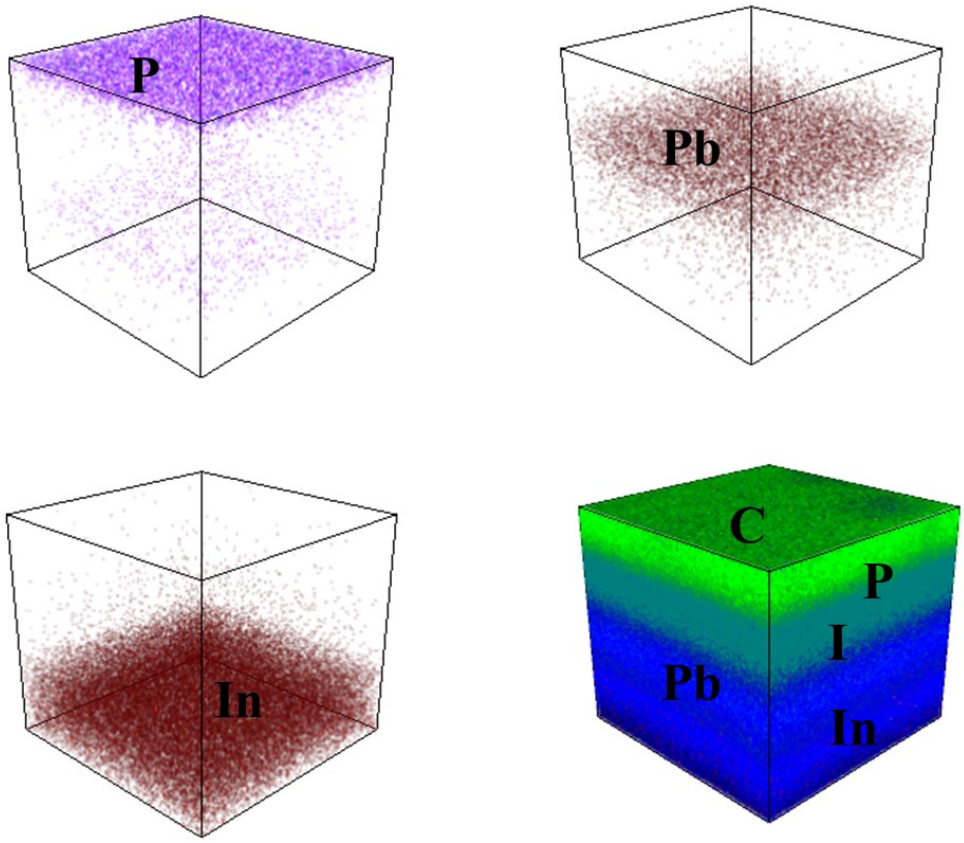

Fig. S1. The TOF-SIMs for depth profiling in ITO/PTAA/$MAPbI_3$/PCBM/DPP/Ag device.

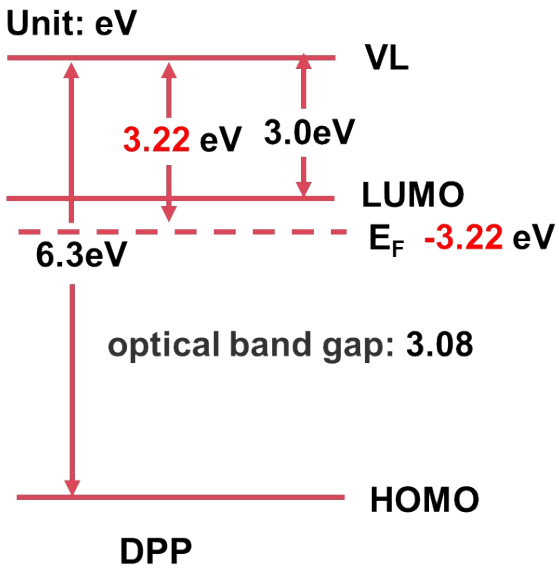

Fig. S2. Energy levels of DPP.

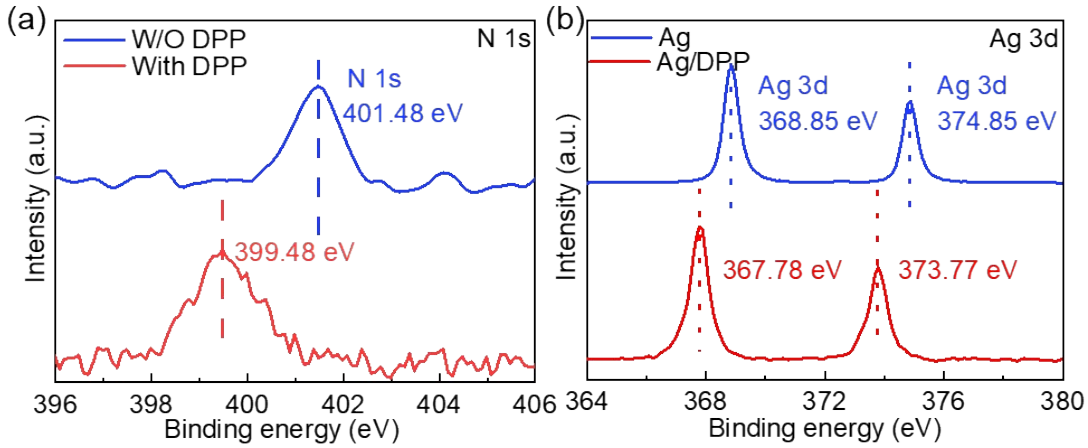

Fig. S3. The XPS of N 1s for ITO/PTAA/$MAPbI_3$ and ITO/PTAA/$MAPbI_3$/DPP films. (b) The XPS of Ag 3d for Ag and DPP/Ag films.

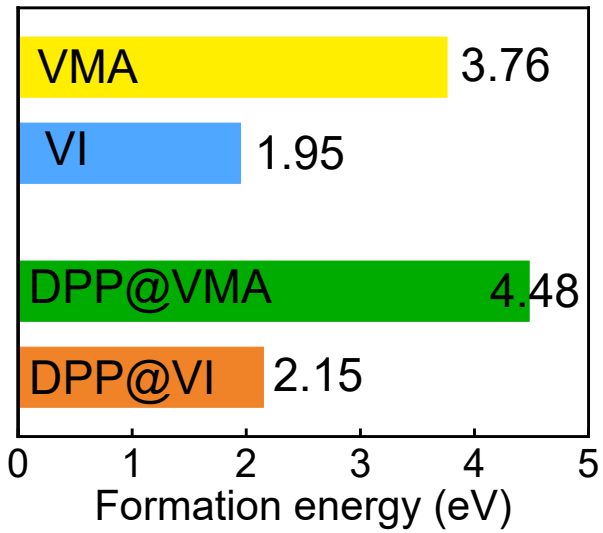

Fig. S4. Formation energy of of MA and I vacancy defects.

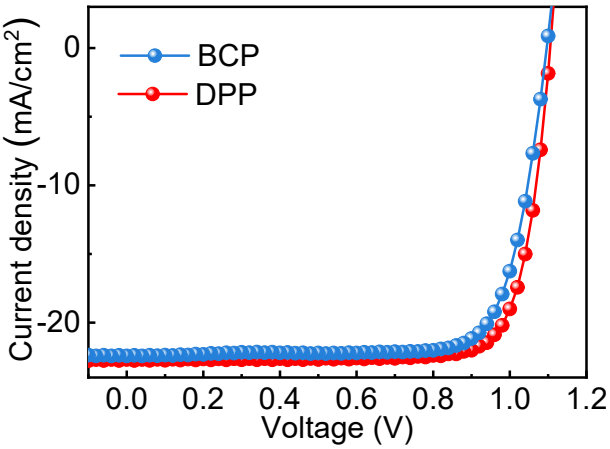

Fig. S5. The J-V curves of the typical BCP device and DPP device.

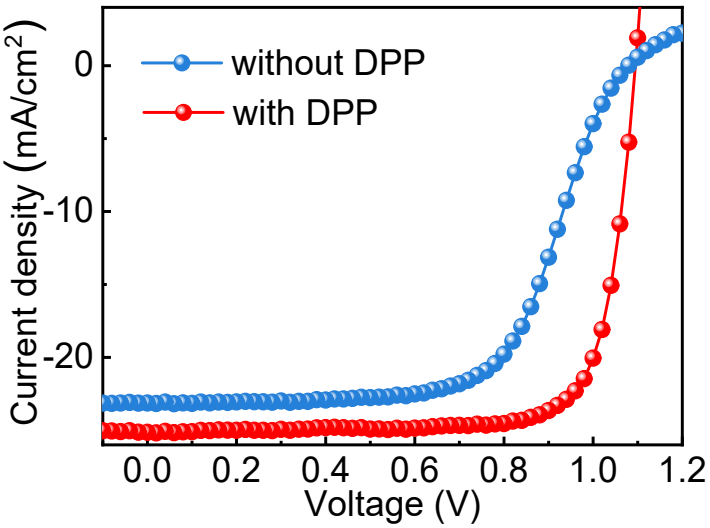

Fig. S6 The J-V curves of the typical inverted PSCs based on $Cs_{0.15}FA_{0.85}Pb(I_{0.95}Br_{0.05})_3$ perovskite composition with and without DPP.

Table S1 The fitting parameters of TRPL spectra of quartz/$MAPbI_3$, quartz/$MAPbI_3$/PCBM and quartz/$MAPbI_3$/PCBM/DPP films.

sample	τ_1 (ns)	A_1 (%)	τ_2 (ns)	A_2 (%)	T_{ave} (ns)
$MAPbI_3$	15.01	50.69	127.72	49.31	178.83
$MAPbI_3$/PCBM	2.48	97.50	9.92	2.50	2.67
$MAPbI_3$/PCBM/DPP	2.39	99.74	8.98	0.26	2.38

Table S2 The average parameters of the BCP and DPP PSCs derived from 10 individual devices. The parameters of the best devices are shown in bracket.

Sample	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
BCP	1.092±0.02 (1.096)	21.66±2.21 (22.43)	77.76±2.54 (77.63)	18.40±1.92 (19.09)
DPP	1.105±0.035 (1.110)	22.21±1.47 (22.69)	79.42±4.25 (80.46)	19.53±0.64 (20.17)

Table S3. The hysteresis of the control and DPP devices from Figure 5d.

Sample	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
Control-F	1.070	19.60	71.35	14.94
Control-R	1.064	18.86	67.32	13.51
DPP-F	1.090	22.02	80.80	19.39
DPP-R	1.081	21.76	79.05	18.61

Table S4 The average parameters of the inverted PSCs based on $Cs_{0.15}FA_{0.85}Pb(I_{0.95}Br_{0.05})_3$ perovskite composition with and without DPP based on 10 individual devices. The parameters of the best devices are shown in bracket.

Sample	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
Without DPP	1.071±0.07 (1.079)	21.75±4.03 (23.14)	59.38±4.60 (63.81)	13.82±3.34 (15.93)
With DPP	1.096±0.004 (1.095)	24.39±0.75 (25.14)	76.67±1.91 (78.16)	20.50±1.01 (21.51)

Table S5. The EIS fitting parameters of control and DPP devices.

Sample	Rs (Ω)	R_{rec} (Ω)	CPE1 (F)	R_{dr} (Ω)	CPE2 (F)
Control	67.33	28460	3.66×10^{-9}	1.03×10^{5}	1.89×10^{-7}
DPP	94.85	31930	4.33×10^{-9}	1.08×10^{5}	1.29×10^{-7}