Hysteresis-free perovskite transistor with exceptional stability through molecular cross-linking and amine-based surface passivation

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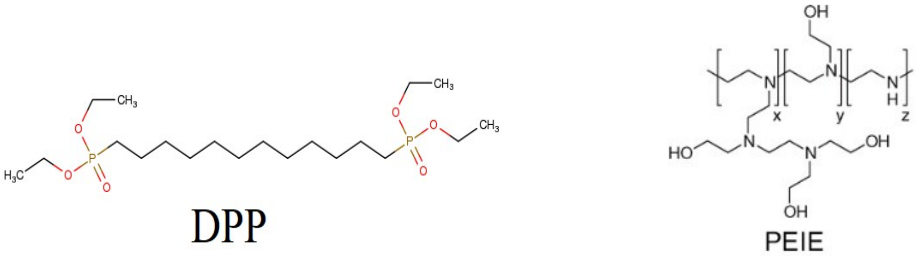


Figure S1. The chemical structure of DPP molecular cross-linker (left) and of PEIE (right) used for surface passivation.

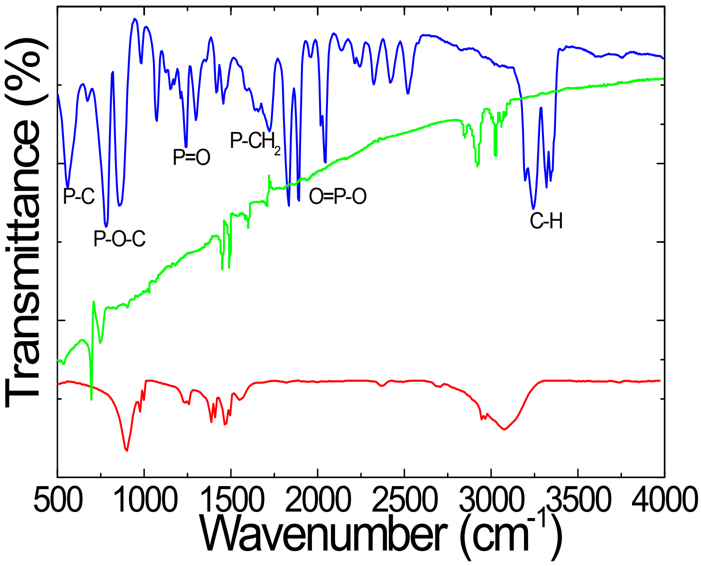


Figure S2. Fourier transform infrared (FTIR) spectra of DPP (blue), CsMAFA (red) and modified-CsMAFA (green) films illustrating significant downward shifts in the FTIR bands of DPP molecules when added into the perovskite precursor solution.

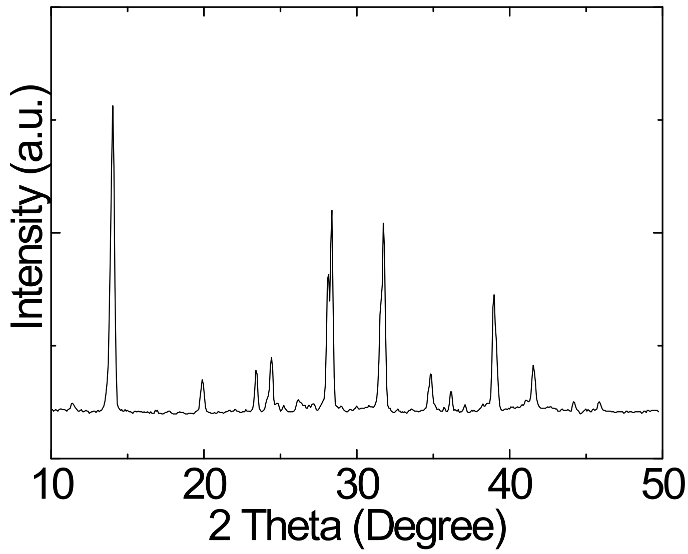


Figure S3. Powder X-ray diffraction (PXRD) pattern of the DPP-modified perovskite material.

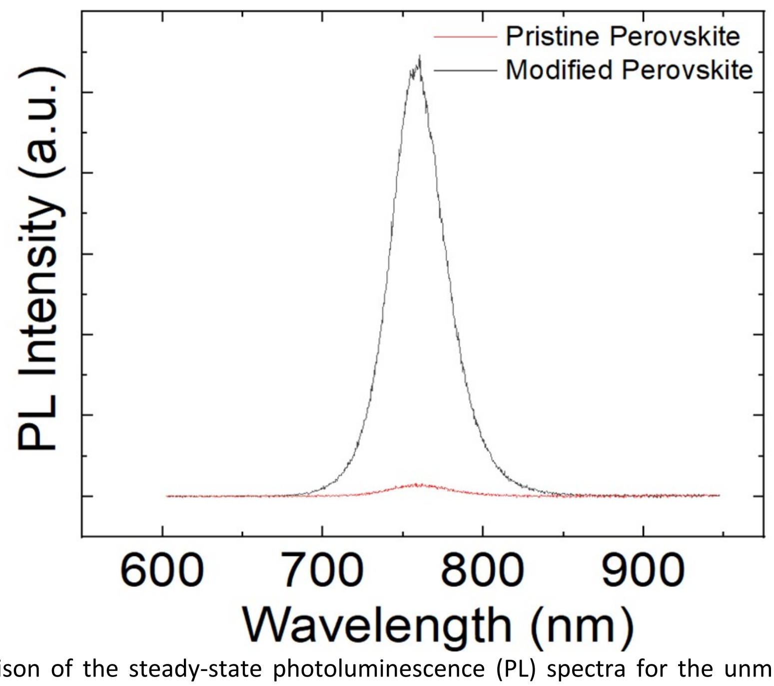


Figure S4. Comparison of the steady-state photoluminescence (PL) spectra for the unmodified-CsMAFA and DPP modified-CsMAFA films deposited on a SiO_2/Si substrate.

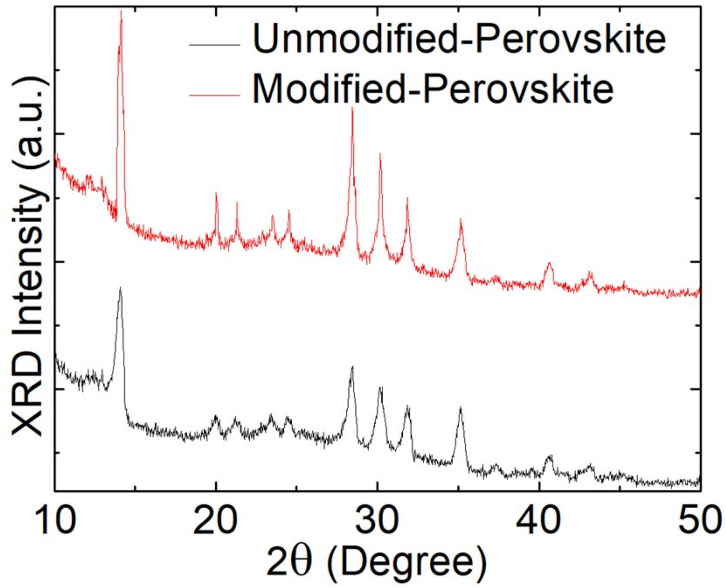


Figure S5. XRD patterns of DPP modified-CsMAFA and unmodified-CsMAFA films.

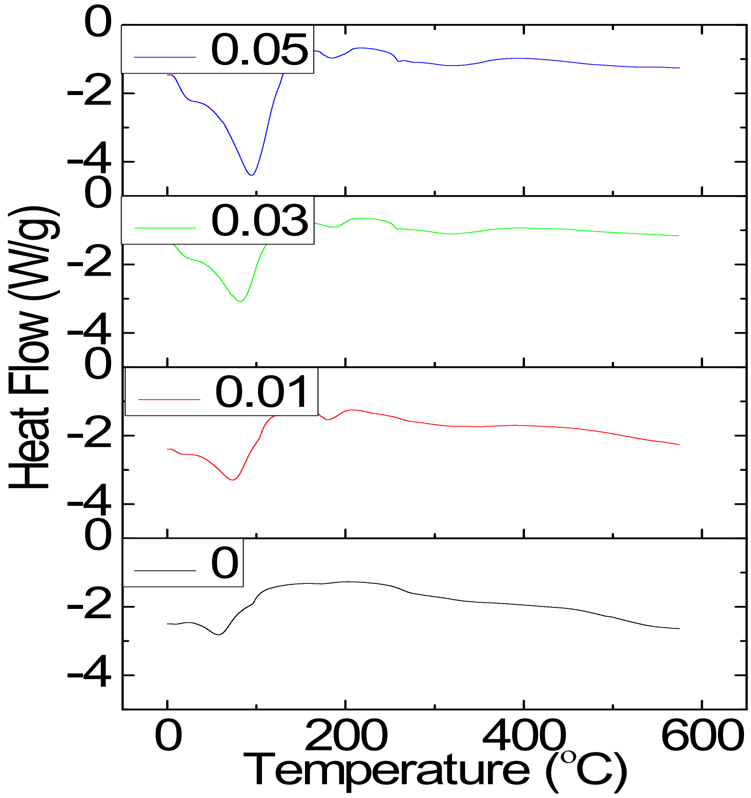
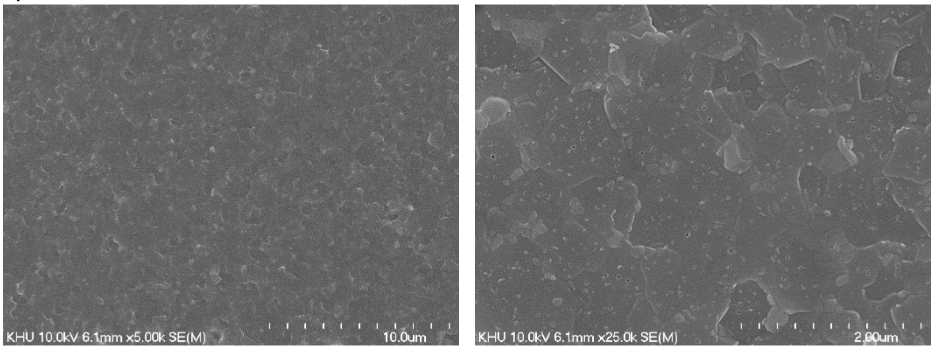
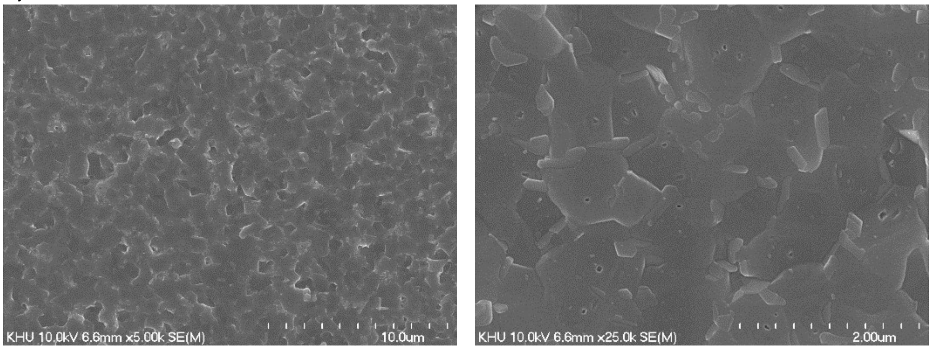


Figure S6. Differential scanning calorimetry of modified $DPP_{(x)}$-$CsMAFA_{(1-x)}$ (x=0, 0.01, 0.03, and 0.05) samples.

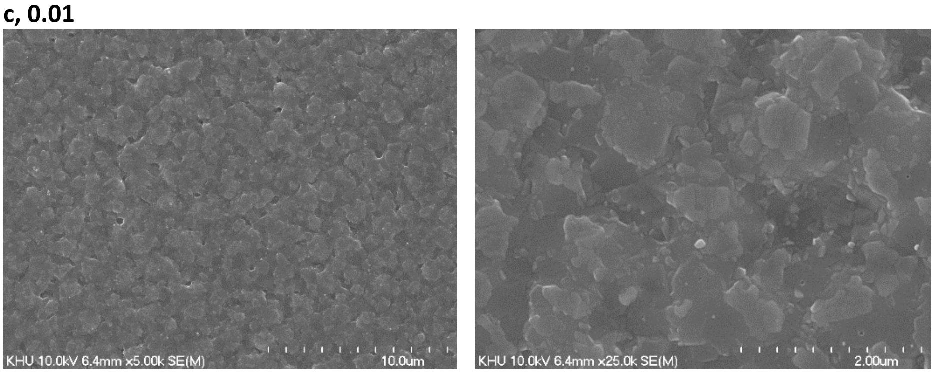
a, 0.05



b, 0.03



c, 0.01



d, 0

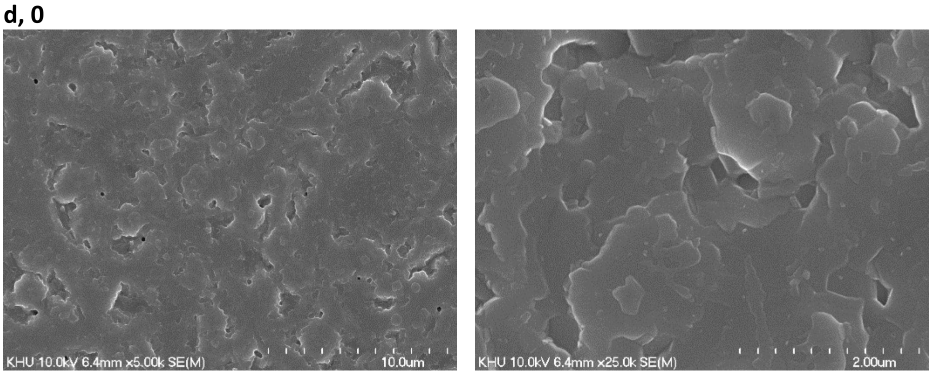


Figure S7. Comparison of the morphology for the (a-c) modified- ($DPP_{(x)}$-$CsMAFA_{(1-x)}$ (x=0, 0.01, 0.03, and 0.05)) and unmodified- (d) CsMAFA films deposited on SiO_2/Si substartes. Dense films with fully coverage on the substrates were only achieved by spin-coating the modified-CsMAFA solutions.

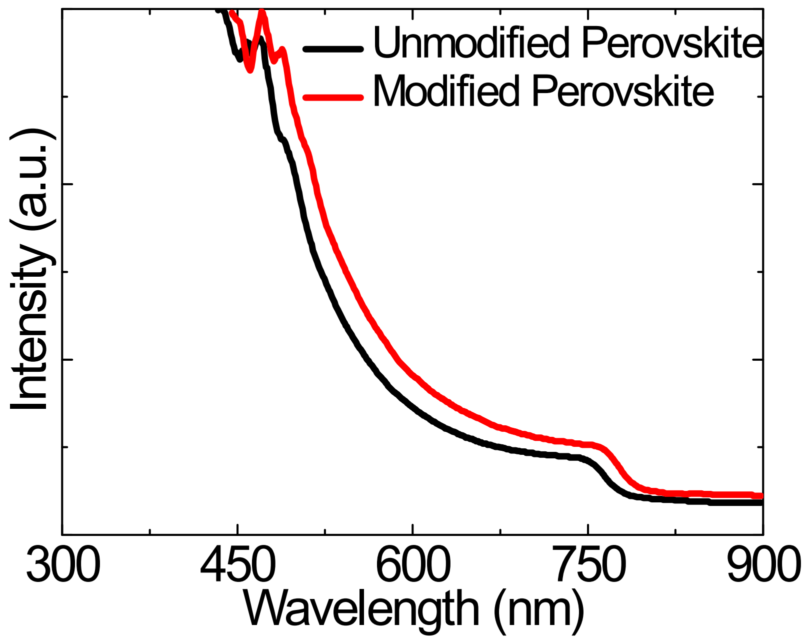


Figure S8. UV-Vis absorption spectra of the unmodified-CsMAFA and DPP modified-CsMAFA films. The red shift of the absorption onset of the DPP-modified film indicates a reduction in the optical bandgap value of the perovskite material (from 1.58 to 1.53 eV) which was also theoretically predicted.

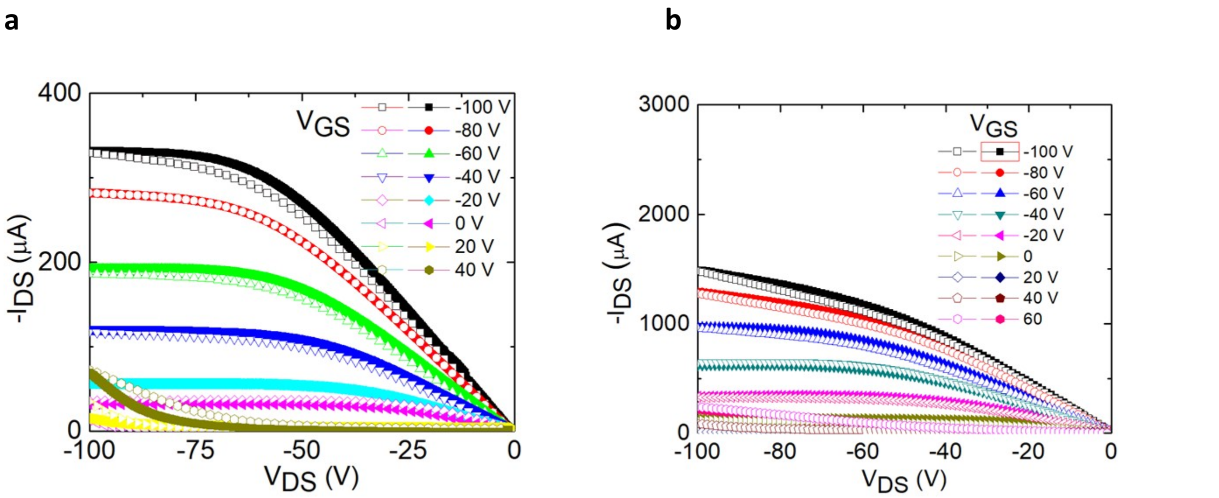


Figure S9. Performance characteristics of the unmodified and DPP modified perovskite FETs on hole operation**.** Hole output characteristics of (a) unmodified and (b) DPP modified-CsMAFA FETs for different V_{GS} measured at room temperature.

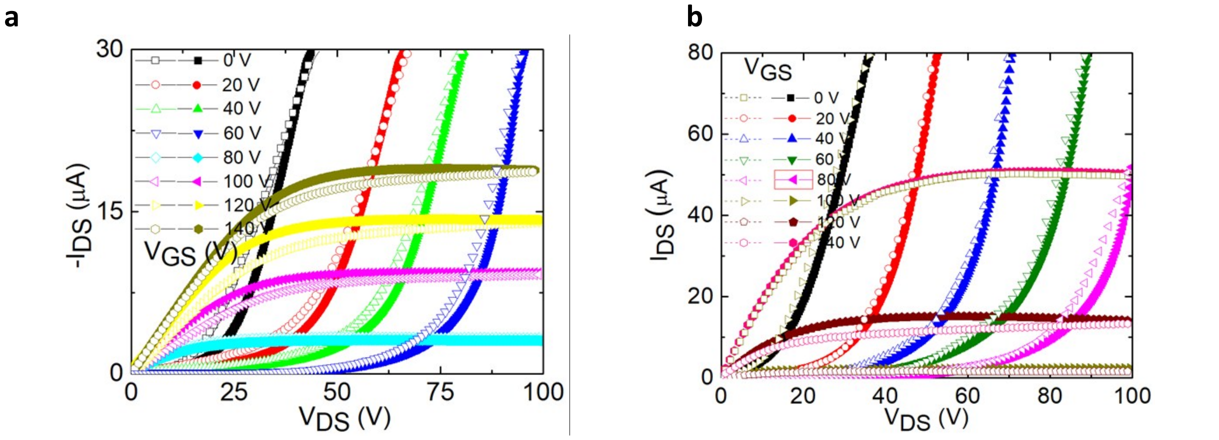


Figure S10. Performance characteristics of the unmodified and DPP modified perovskite FETs on electron operation. Electron output characteristics of (a) unmodified and (b) DPP modified-CsMAFA FETs for different V_{GS} measured at room temperature.

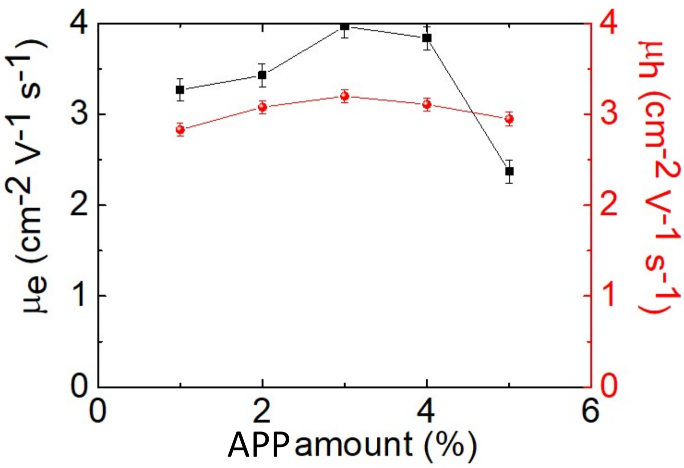


Figure S11. The room temperature μ_h and μ_e variations as a function of DPP amount.

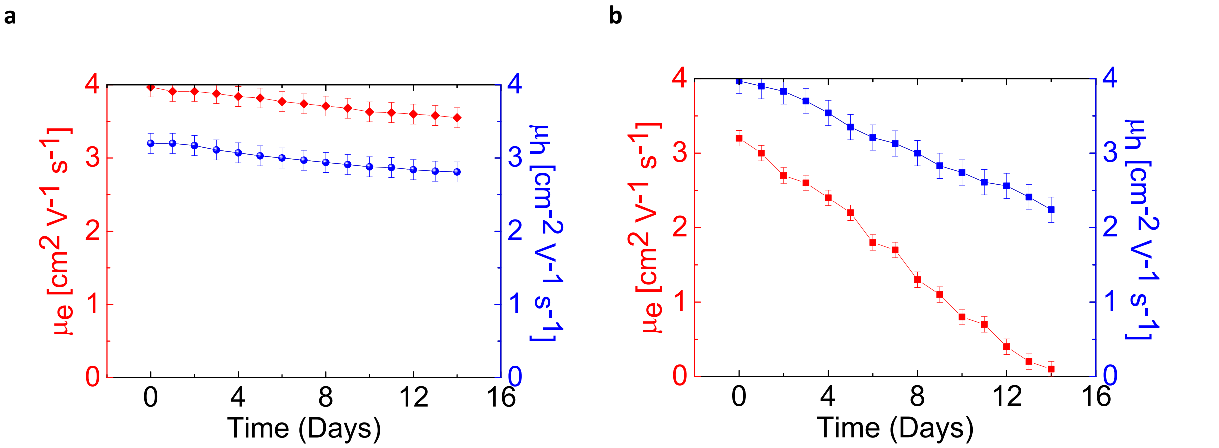


Figure S12. The room temperature hole and electron mobilities versus time for both (a) modified- and (b) unmodified-CsMAFA.

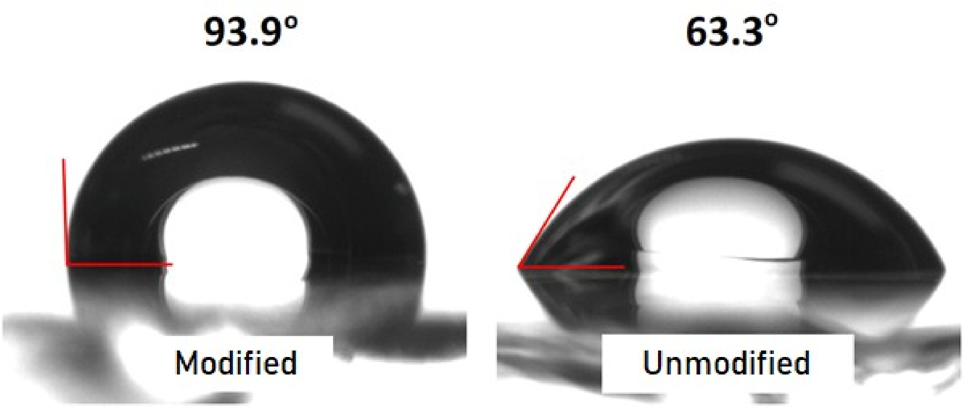


Figure S13. The contact angles of water on modified-CsMAFA film (left) and on unmodified-CsMAFA film (right).

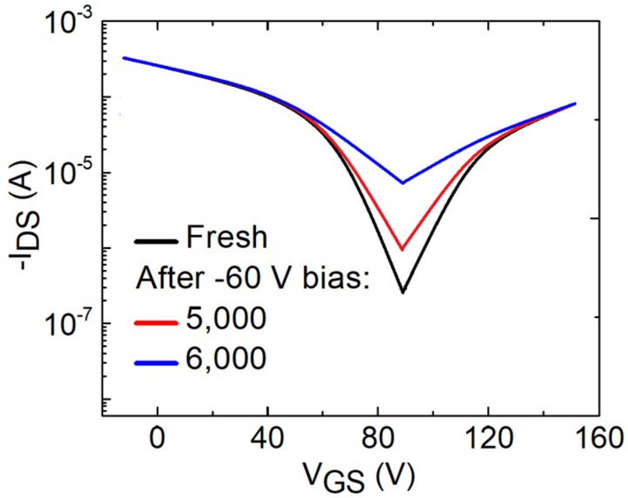


Figure S14. Variation of the channel current (I_{SD}-V_{GS}) under a continuous bias stress of -20 V for different times up to 6,000 s.

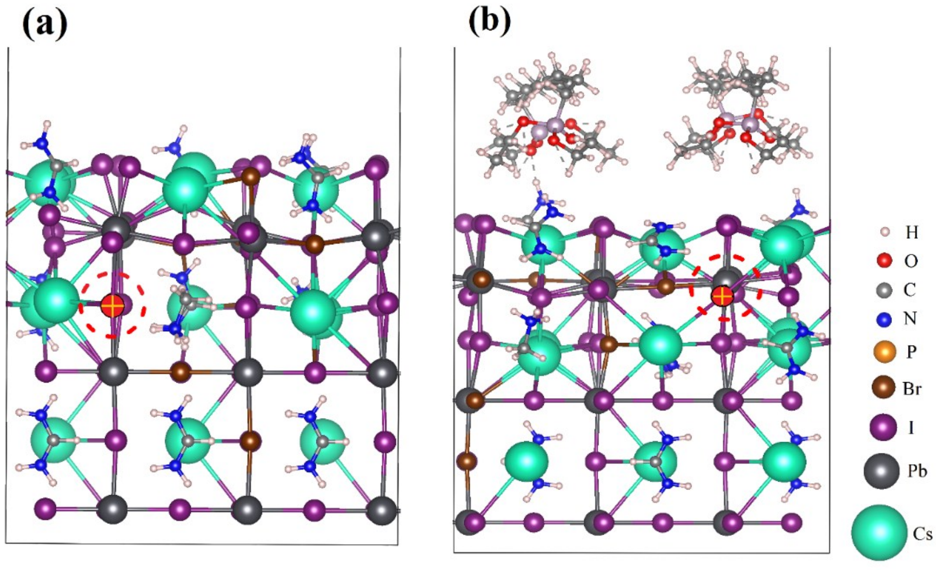


Figure S15. Optimized stable geometrical structure with 2% I vacancy of (a) unmodified-CsMAFA and (b) and modified-CsMAFA. The red circles show the iodide vacancy.

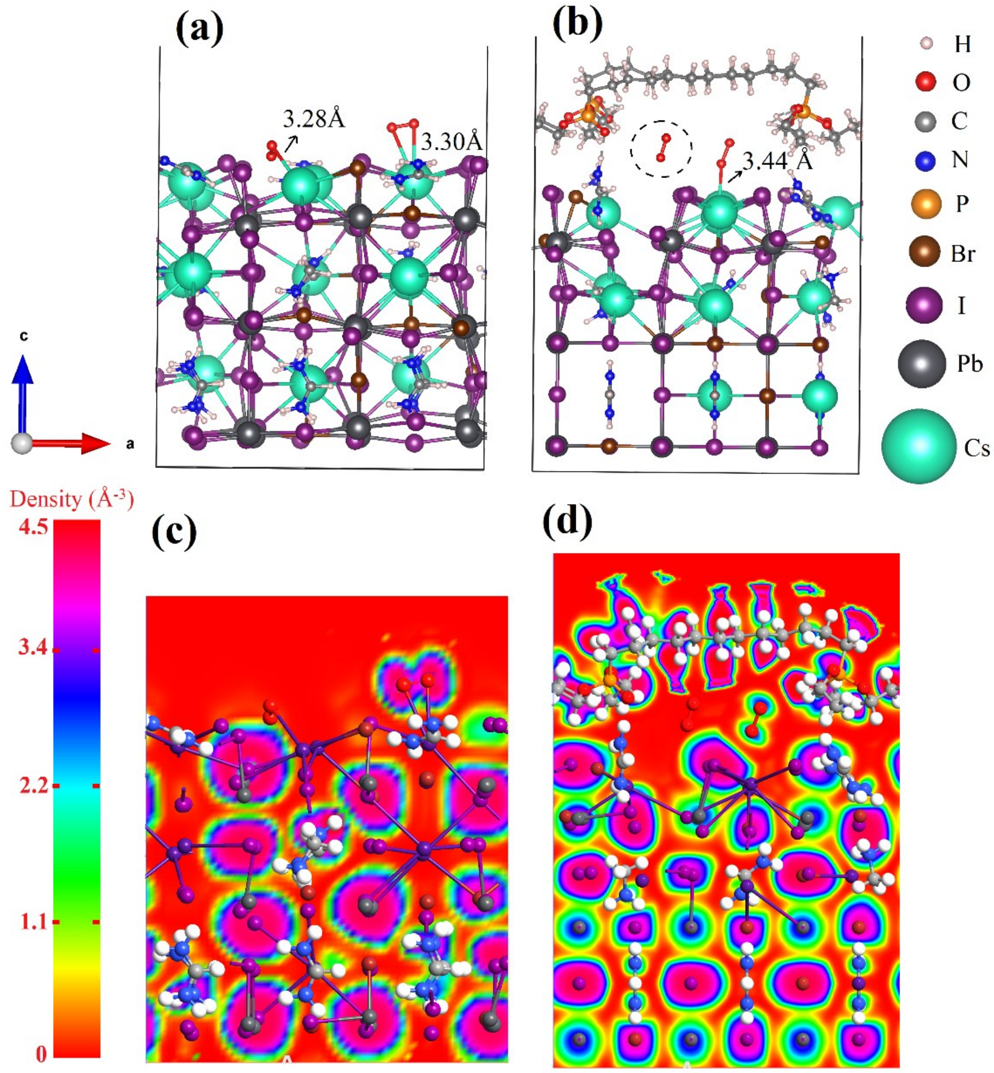


Figure S16. Optimized relaxed structure of (a) unmodified-CsMAFA@O_2, where the oxygen molecules are attached to Cs surface atoms at about 3.30 Å. (b) Optimized structure of modified-CsMAFA@O_2, where two oxygen molecules are inserted between crosslinker and perovskite surface; one of the oxygen atoms interacts with Cs surface atom at about 3.44 Å above the perovskite surface. Electronic total charge density slices of the (c) O_2 adsorbed on unmodified-CsMAFA and (d) O_2 adsorbed on modified-CsMAFA.

Table S1. Summary of glass transition temperatures for modified-CsMAFA with different crosslinker amounts.

Crosslinker	Perovskite composition	T_g (˚C)
0	100	58.6
0.01	0.99	74.5
0.03	0.97	80.8
0.05	0.96	94.1

Table S2 Simulated total energy of unmodified-CsMAFA, modified-CsMAFA, DPP, water, O_2, and per molecule water and oxygen adsorption energy on the surface of unmodified-CsMAFA and modified-CsMAFA.

Species	Total Energy (eV)	Adsorption Energy (kcal mol^{-1})
Unmodified-CsMAFA	-55993.3897	
Modified-CsMAFA	-69995.7738	**-48.20**
DPP	-6999.1015	
Water	-466.8687	
Oxygen molecule	-860.5647	
Unmodified-CsMAFA@H_2O	-56936.4168	**-107**
Unmodified-CsMAFA@O_2	-57739.3709	**-286.53**
Modified-CsMAFA@H_2O	-70932.6866	**-36.44**
Modified-CsMAFA@O_2	-71725.9399	**-104.58**

Table S3. DFT simulated valence band maximum (VBM), conduction band minimum (CBM), band gap, and effective masses of photogenerated electrons and holes. Effective masses of electrons and holes are estimated from the calculated band structure of CBM and VBM, respectively.

Species	Direction in Brillouin zone	m_e*/m_0 (m_e)	m_h*/m_0 (m_e)	VB (eV)	CB (eV)	Band gap (eV)
Unmodified-CsMAFA	**C**	**2.98**	**0.15**	**-0.79**	**0.79**	**1.58**
	L	**2.98**	**0.15**	**-0.79**	**0.79**	**1.58**
	Y	2.94	5.25	-0.93	0.79	1.72
	B	1.00	0.14	-0.84	1.04	1.88
	X	1.00	0.14	-0.84	1.04	1.88
Modified-CsMAFA	U	0.16	12.24	-0.88	0.72	1.60
	V	**0.16**	**0.72**	**-0.73**	**0.71**	**1.44**
	R	**0.16**	**0.72**	**-0.73**	**0.71**	**1.44**
	X	0.16	12.24	-0.88	0.72	1.60
	Y	0.16	0.93	-0.78	0.98	1.76
	T	0.16	0.93	-0.78	0.98	1.76

Table S4. FETs performance of unmodified-CsMAFA. The *p*-channel and *n*-channel characteristics of ambipolar FETs were measured with V_{DS} = −100 and 100 V, respectively. (*L* = 50 μm and *W* = 1000 μm).

Condition	p-channel				n-channel			
T_a [ºC]	$\mu_{h,max}$ [cm² V⁻¹ s⁻¹]	$\mu_{h,avg}$ [cm² V⁻¹ s⁻¹]	I_{on}/I_{off}	V_t [V]	$\mu_{e,max}$ [cm² V⁻¹ s⁻¹]	$\mu_{e,avg}$ [cm² V⁻¹ s⁻¹]	I_{on}/I_{off}	V_t [V]
RT	0.16	0.08 (±0.04)	>10^5	4	3 x 10^{-2}	2 x 10^{-2} (±0.003)	>10^3	84
50	0.52	0.47 (±0.03)	>10^6	10	0.18	0.13 (±0.02)	>10^3	102
100	2.21	2.19 (±0.14)	>10^5	-9	0.38	0.33 (±0.13)	>10^3	80
150	1.31	1.35 (±0.16)	>10^6	2	0.18	0.12 (±0.03)	>10^4	94

Table S5. Performance parameters of FETs based on of DPP modified-CsMAFA. The *p*-channel and *n*-channel characteristics of ambipolar FETs were measured with V_{DS} = −100 and 100 V, respectively. (*L* = 50 μm and *W* = 1000 μm).

Condition	p-channel				n-channel			
T_a [ºC]	$\mu_{h,max}$ [cm² V⁻¹ s⁻¹]	$\mu_{h,avg}$ [cm² V⁻¹ s⁻¹]	I_{on}/I_{off}	V_t [V]	$\mu_{e,max}$ [cm² V⁻¹ s⁻¹]	$\mu_{e,avg}$ [cm² V⁻¹ s⁻¹]	I_{on}/I_{off}	V_t [V]
RT	3.16	2.87 (±0.26)	>10^5	4	2.37	0.18 (±0.10)	>10^2	84
50	3.23	3.16 (±0.17)	>10^6	10	2.79	0.65 (±0.13)	>10^4	102
100	3.97	3.48 (±0.30)	>10^4	-9	3.20	3.17 (±0.20)	>10	80
150	2.27	1.99 (±0.25)	>10^4	2	2.21	0.93 (±0.33)	>10^2	94

Table S6. Performance summary of DPP modified and PEIE treated FETS. The *p*-channel and *n*-channel characteristics of ambipolar FETs were measured with V_{DS} = −100 and 100 V, respectively. (*L* = 50 μm and *W* = 1000 μm).

Condition	*p*-channel				*n*-channel			
T_a [ºC]	$\mu_{h,max}$ [cm² V⁻¹ s⁻¹]	$\mu_{h,avg}$ [cm² V⁻¹ s⁻¹]	I_{on}/I_{off}	V_t [V]	$\mu_{e,max}$ [cm² V⁻¹ s⁻¹]	$\mu_{e,avg}$ [cm² V⁻¹ s⁻¹]	I_{on}/I_{off}	V_t [V]
N/A	3.21	2.92 (±0.11)	>10^5	3	2.42	0.23 (±0.10)	>10^2	81
50	3.31	3.18 (±0.12)	>10^6	11	2.84	0.74 (±0.16)	>10^4	105
100	4.02	3.52 (±0.22)	>10^4	-7	3.35	3.25 (±0.13)	>10	82
150	2.32	2.04 (±0.11)	>10^4	3	2.26	0.98 (±0.15)	>10^2	94

Table S7. The state-of-art atmospheric conditions measured perovskite FET characteristics reported.

Material	Hole mobility ($cm^2 V^{-1} s^{-1}$)	Electron mobility ($cm^2 V^{-1} s^{-1}$)	Subthreshold Swing (Holes/electrons) ($mV dec^{-1}$)	Hysteresis	Ref.
$CH_3NH_3PbI_3$	$5x10^{-4}$	10^{-4}	-	Yes	[2]
$CH_3NH_3PbI_3$	0.18	0.17	-	Yes	[3]
$CH_3NH_3PbI_{3-x}Cl_x$	1.24	1.01	-	Yes	[3]
CH3NH3$PbI_{3-x}Cl_x$	1.3	1.0	2100/1500	Yes	[4]
$Cs_x(MA_{0.17}FA_{0.83})_{1-x}Pb(Br_{0.17}I_{0.83})_3$	2.02	2.39	-	Yes	[5]
$CH_3NH_3PbI_3$	-	0.05	-	Yes	[6]
$CsPbBr_3$	0.32	-		Yes	[7]
$(PEA)_2SnI_4$	0.33	-	7100	Yes	[8]
$Cs_x(MA_{0.17}FA_{0.83})_{1-x}Pb(Br_{0.17}I_{0.83})_3$	**4.02**	**3.35**	**288/267**	**No**	**This work**

Table S8. Formation energies of defective unmodified-CsMAFA and modified-CsMAFA; 2% Iodide vacancy was created in both species.

Species	Formation Energy (eV)
Unmodified-CsMAFA	2.41
Modified-CsMAFA	2.87

Table S9. Relaxed fractional coordinates of unmodified-CsMAFA.

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