Supplementary materials

The influence of different recombination pathways on hysteresis in perovskite solar

cells with ion migration

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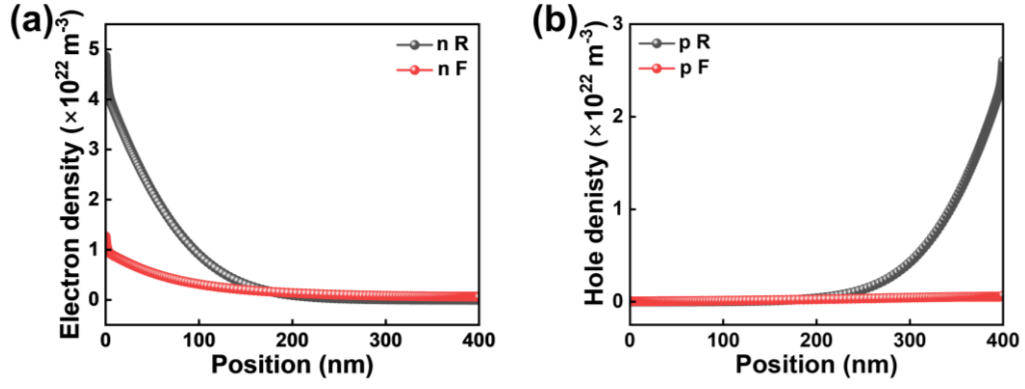
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Figure S1. Charge carrier distribution in perovskite layers of different voltage scanning direction: (a) electrons; (b) holes.
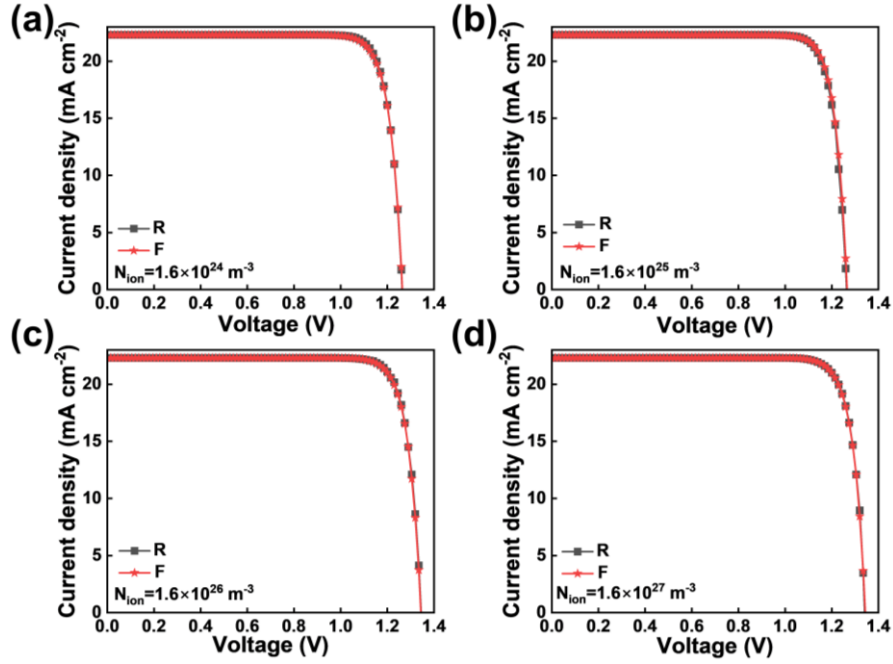

Figure S2. The simulation of *J-V* curves for PSCs with same negligible recombination and with different density of mobile ions: (a) 1.6×10^{24} m^{-3}; (b) 1.6×10^{25} m^{-3}; (c) 1.6×10^{26} m^{-3}; (d) 1.6×10^{27} m^{-3}.
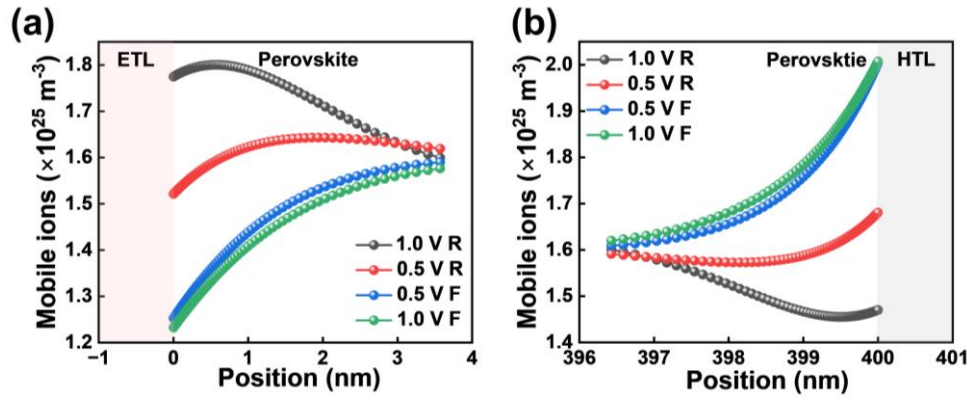
Figure S3. The distribution of mobile ions at different voltages near the interface between charge transporting layers and perovskite films. The density of mobile ions for the simulation is 1.6×10^{25} m^{-3}. (a) ETL/Perovskite interface; (b) HTL/Perovskite interface.
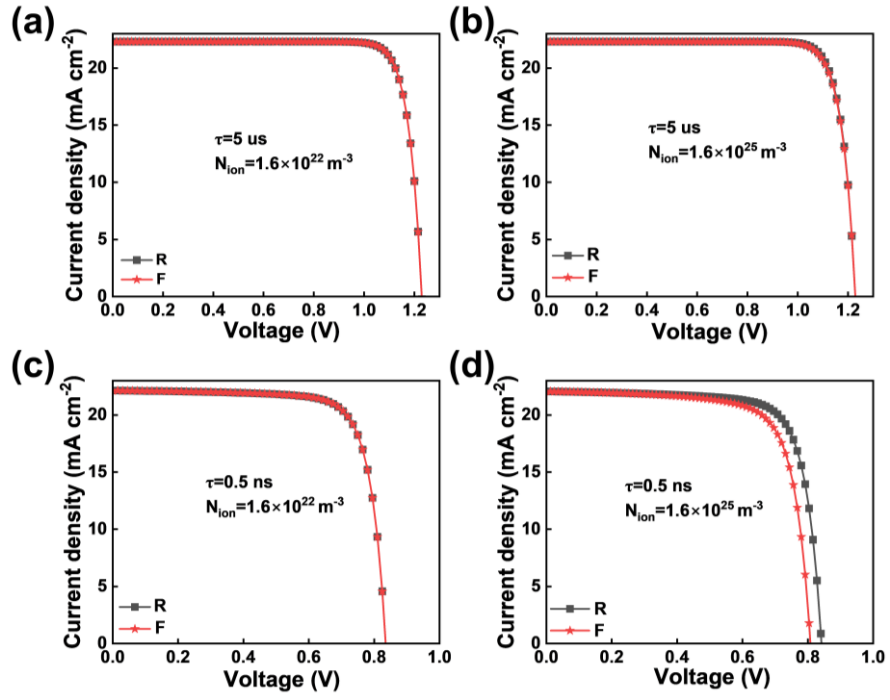
Figure S4. (a) *J-V* curves for a PSC with negligible bulk recombination and negligible density of mobile ions; (b) *J-V* curves for a PSC with negligible bulk recombination and high density of mobile ions; (c) *J-V* curves for a PSC with severe bulk recombination and negligible density of mobile ions; (d) *J-V* curves for a PSC with severe bulk recombination and high density of mobile ions.
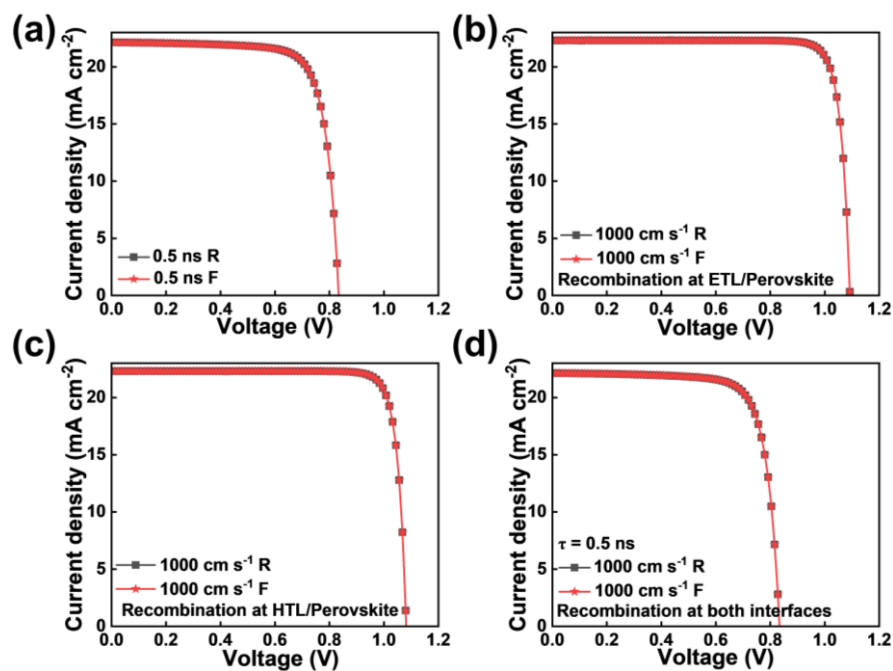
Figure S5. (a) only severe bulk recombination coupling with negligible ion migration; (b) only severe interface recombination at ETL/perovskite interface coupling with negligible ion migration; (c) only severe interface recombination at HTL/perovskite interface coupling with negligible ion migration; (d) severe bulk recombination with severe interface recombination at both interfaces coupled with negligible ion migration.
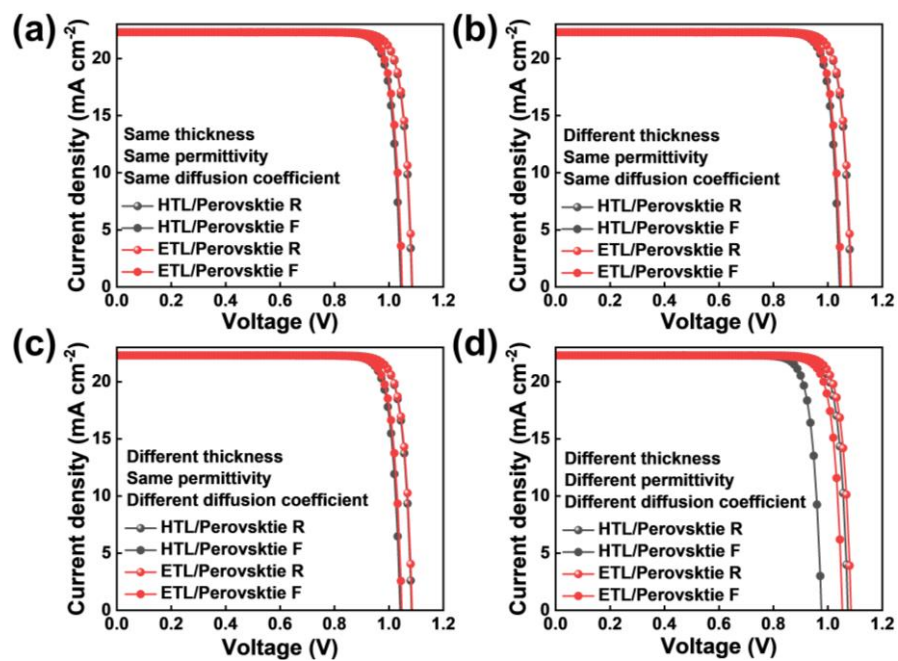
Figure S6. *J-V* curves for interface recombination at ETL/Perovskite and HTL/Perovskite interface respectively: (a) same thickness, same permittivity and same diffusion coefficient for transporting layers; (b) different thickness, same permittivity and same diffusion coefficient for transporting layers; (c) different thickness, same permittivity and same diffusion coefficient for transporting layers; (d) different thickness, same permittivity and same diffusion coefficient for transporting layers.

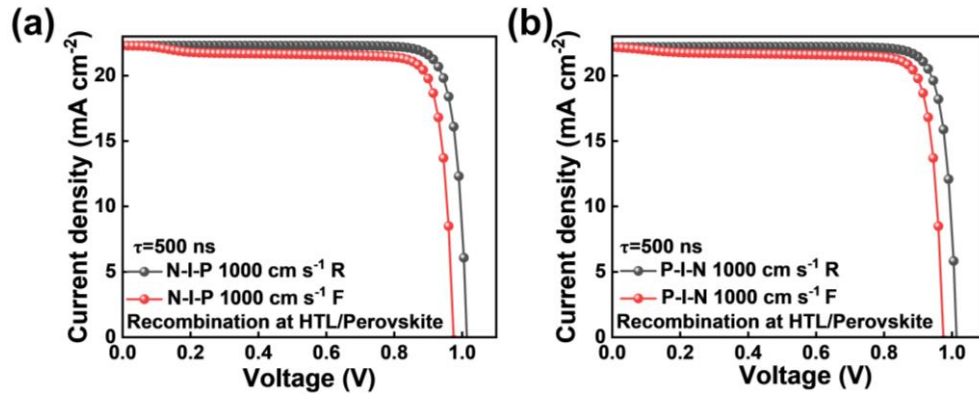**Figure S7.** *J-V* curves for both N-I-P and P-I-N PSCs under same condition: (a) N-I-P; (b) P-I-N.
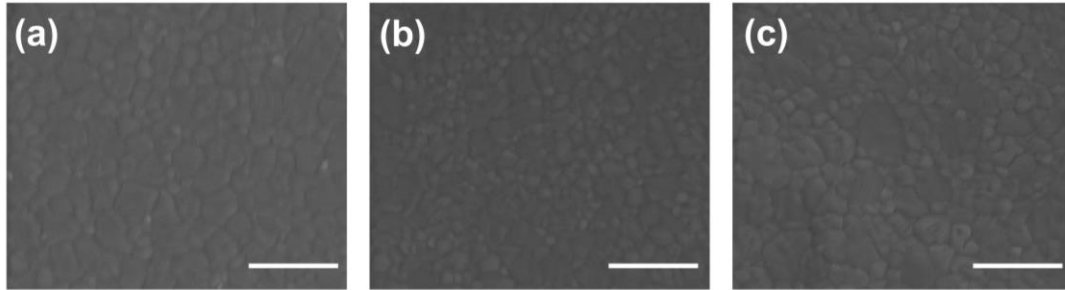

Figure S8. SEM images for the perovskite films on different substrates. (a) SnO_2; (b) SnO_2 NC;

(c) TiO_2. The scale bar is 1 μm.

Figure S9. (a) TRPL data for perovskite films with the structure of glass/MAPbI$_3$. (b) Urbach

energy for perovskite films with the structure of glass/MAPbI$_3$.
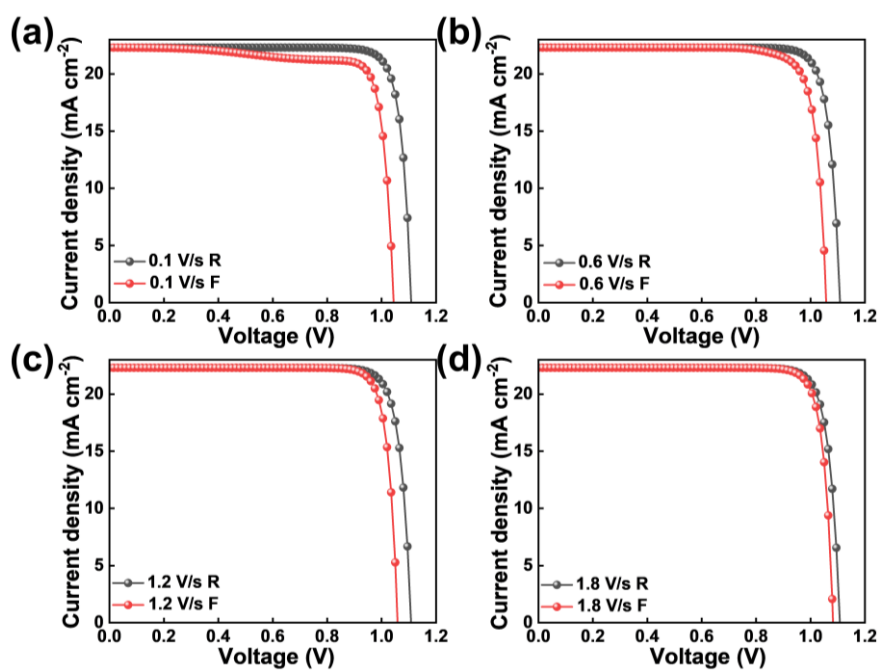
Figure S10. The effect of scan rates on hysteresis in PSCs. The carrier lifetime is 500 ns. The interface recombination velocity is 100 cm/s for both holes and electrons at both ETL/Perovskite and HTL/Perovskite interface. (a) 0.1 V/s; (b) 0.6 V/s; (c) 1.2 V/s; (d) 1.8 V/s.

Table S1. Device parameters used for simulations

Parameter	Symbol	Value	Unit
Thickness of HTL	d_{HTL}	200	nm
Thickness of perovskite	d_{pero}	400	nm
Thickness of ETL	d_{ETL}	100	nm
Valence band maximum of HTL	$E_{V,HTL}$	−5.4	eV
Conduction band minimum of perovskite	$E_{C,pero}$	−3.9	eV
Valence band maximum of Perovskite	$E_{V,pero}$	−5.4	eV
Conduction band minimum of ETL	$E_{C,ETL}$	−3.9	eV
Relative dielectric constant of HTL	ϵ_{HTL}	3	/
Relative dielectric constant of perovskite	ϵ_{pero}	24.1	/
Relative dielectric constant of ETL	ϵ_{ETL}	10	/
Effective density of states in HTL	$N_{C/V,HTL}$	5×10^{25}	m^{-3}
Effective conduction band density of states in perovskite	$N_{C,pero}$	8.1×10^{24}	m^{-3}
Effective valence band density of states in perovskite	$N_{V,pero}$	5.8×10^{24}	m^{-3}
Effective density of states in ETL	$N_{C/V,ETL}$	5×10^{25}	m^{-3}
Hole diffusion coefficient in HTL	$D_{h,HTL}$	1×10^{-6}	m^{2}s^{-1}
Hole diffusion coefficient in perovskite	$D_{h,pero}$	1.7×10^{-4}	m^{2}s^{-1}
Electron diffusion coefficient in perovskite	$D_{e,pero}$	1.7×10^{-4}	m^{2}s^{-1}
Electron diffusion coefficient in ETL	$D_{e,ETL}$	1×10^{-5}	m^{2}s^{-1}
Effective doping density in HTL	$N_{A,,HTL}$	1×10^{24}	m^{-3}
Effective doping density in ETL	$N_{D,ETL}$	1×10^{24}	m^{-3}
Density of ion vacancy	N_{ion}	1.6×10^{25}	m^{-3}
Ion migration activation energy	E_a	0.5	eV
Temperature	T	298	K

The charge carrier lifetime can be fitted according to a biexponential decay function: $I = A_1 \exp\left(-\frac{t}{\tau_1}\right) + A_2 \exp\left(-\frac{t}{\tau_2}\right)$ (Where I is the intensity of photoluminescence. τ_1 and τ_2 are the fast and slow decay lifetimes. A_1 and A_2 are pre-exponential factors. t is the time.). The fitting results are listed in Table S2.

Table S2. Fitting results of TRPL results.

	A_1	τ_1 (ns)	A_2	τ_2 (ns)
Glass/MAPbI$_3$	0.24	4.27	0.66	56.40