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Minimizing Performance Degradation Induced by Interfacial Recombination in Perovskite Solar Cells through Tailoring of the Transport Layer Electronic Properties—Supplement

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Supplementary Material

Minimizing Performance Degradation Induced by Interfacial Recombination in Perovskite Solar Cells Through Tailoring of the Transport Layer Electronic Properties

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Table S1 Material parameters used for drift-diffusion simulation

Parameters	Symbol (Unit)	Perovskite	$CuCrO_2$	PCBM
Electron affinity	EA (eV)	3.9	variable	4.2
Conduction band effective density of states	$N_{C,}$ (cm^{-3})	2.2×10^{18}	1×10^{19}	1×10^{19}
Valence band effective density of states	$N_{V,}$ (cm^{-3})	1.9×10^{19}	1×10^{19}	1×10^{19}
Radiative recombination coefficient	k (cm^3s^{-1})	2×10^{-10}	/	/
Electron mobility	μ_e ($cm^2V^{-1}s^{-1}$)	1	9×10^{-3}	1×10^{-2}
Hole mobility	μ_h ($cm^2V^{-1}s^{-1}$)	1	9×10^{-3}	1×10^{-2}
Background hole concentration	N_A (cm^{-3})	0	variable	0
Background electron concentration	N_D (cm^{-3})	1×10^{13}	0	5×10^{17}
Relative permittivity	ε (ε_0)	6.5	10	4
Bandgap	E_g (eV)	1.55	3.15	1.8
Electron & hole capture cross section	$\sigma_{n,p}$ (cm^2)	1×10^{-10}	/	/
Interfacial defect energy level	E_t (eV)	midgap	/	/
Total interfacial defect density	N_t (cm^{-3})	variable	/	/
Bulk SRH recombination lifetime	τ (s)	1×10^{-6}	/	/
Surface recombination velocity	$\upsilon_{h,h}$ (cm/s)	10^5		

* The photo-generation is calculated using the Transfer Matrix Method (TMM) based on optical constant for each layer. The optical constant for the perovskite layer is obtained from reference.[1]

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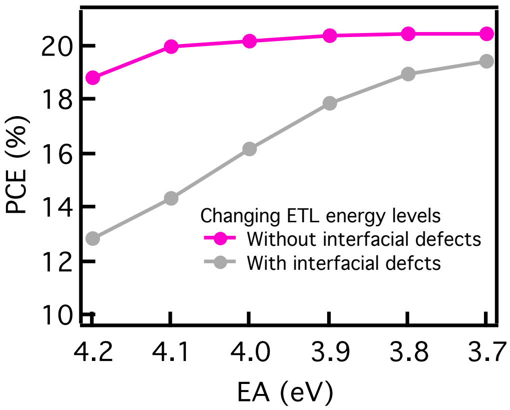

Figure S1 Simulated PCEs for devices with varying EA of PCBM without (magenta circles) and with (grey circles) interfacial defects of a density of 1×10^{11} cm^{-2}.

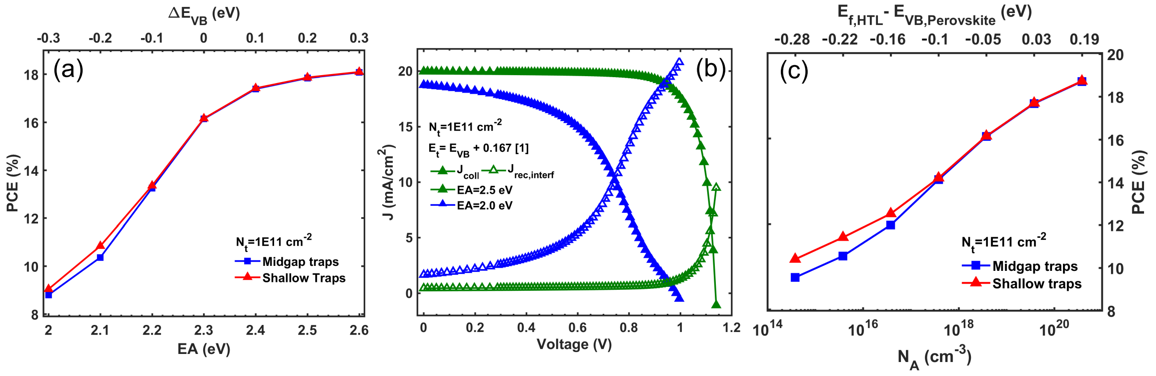

Figure S2 The effect of defect energy position is compared for a deep (mid-gap) defect and a shallow (0.167 eV above the valence band) defect.[2] (a) Simulated PCEs for devices with varying EA with deep defect (blue squares) and shallow defect (red triangles) defects. The corresponding energy difference between the valence band maximum (VBM) of the HTL and the perovskite (ΔE_{VB}) is shown on the top x-axis. The N_A is fixed at 3.8×10^{18} cm^{-3}. (b) Collected current density (J_{coll}) and interfacial recombination current ($J_{rec,interf}$) vs. voltage for shallow defect devices with HTL EA of 2.5 eV (green) and 2 eV (blue) for the shallow defect. (c) Simulated PCEs for devices with varying N_A with mid-gap defect (blue squares) and shallow defect (red triangles). The corresponding energy difference between the Fermi level of the HTL and the VBM of the perovskite ($E_{f,HTL}$ - $E_{VB,perovskite}$) is shown on the top x-axis. The EA is fixed at 2.3 eV. The deep and shallow defects show similar results within the range of simulated EA and N_A.

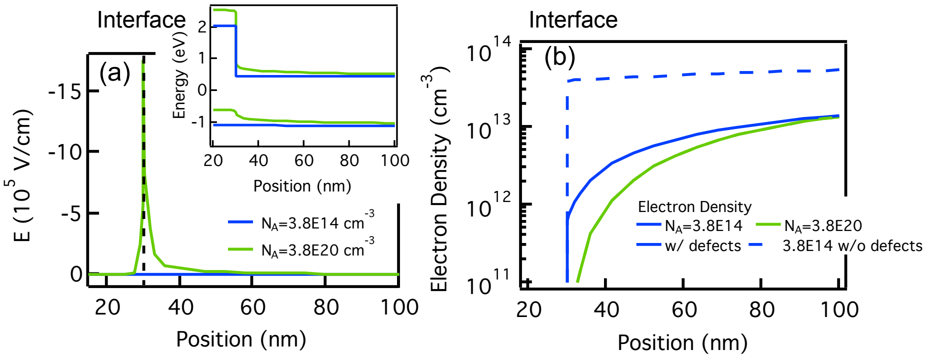

Figure S3 (a) Electrical field vs. position near the HTL-perovskite interface under 1 Sun illumination for the devices with a HTL N$_A$ of 3.8×10^{18} cm^{-3} (green) and 3.8×10^{14} cm^{-3} (blue). The black dashed line indicates the interface position. The inset shows the band diagram near the interface. The electrical field and band alignment are independent of interfacial defect. (b) Electron density vs. position for the device with interfacial defects (N$_t$=1×10^{11} cm^{-2}, solid lines) and without interfacial defects (dashed lines) in the perovskite layer. The color scheme is the same as in (a).

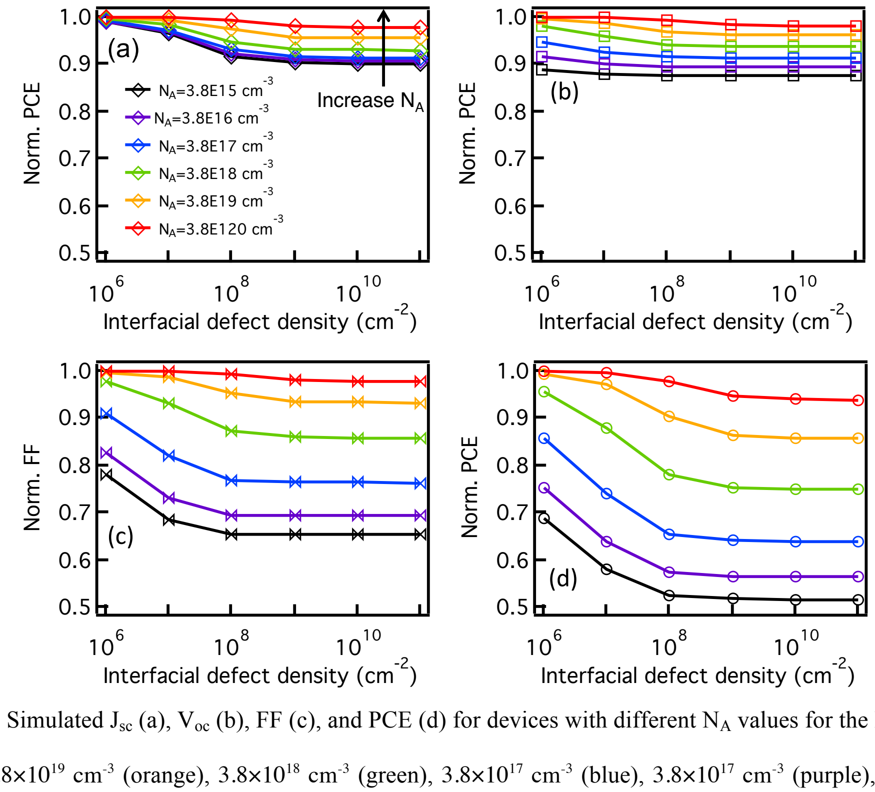

Figure S4 Simulated J$_{sc}$ (a), V$_{oc}$ (b), FF (c), and PCE (d) for devices with different N$_A$ values for the HTL: 3.8×10^{20} cm^{-3} (red), 3.8×10^{19} cm^{-3} (orange), 3.8×10^{18} cm^{-3} (green), 3.8×10^{17} cm^{-3} (blue), 3.8×10^{17} cm^{-3} (purple), and 3.8×10^{16} cm^{-3} (black). The arrow indicates the direction of increasing N$_A$. All parameters are normalized to the values of devices without interfacial defects.

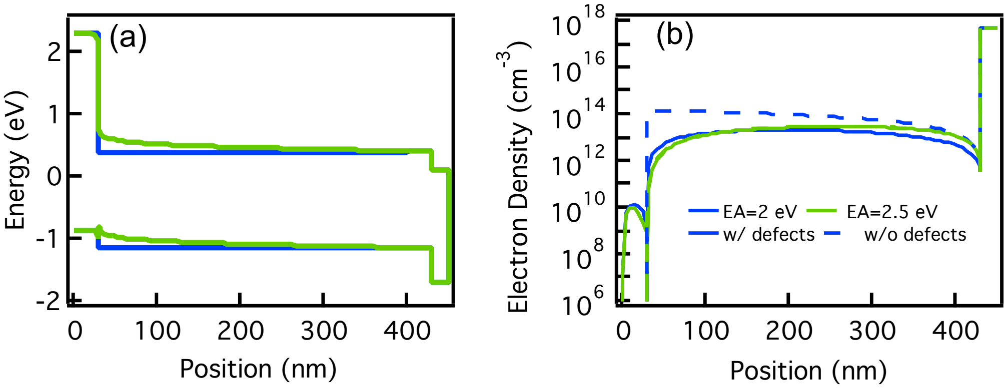

Figure S5 Band diagram (a) and electron density distribution (b) across the entire device under 1 Sun illumination for the devices with a HTL EA of 2.5 eV (green) and 2 eV (blue).

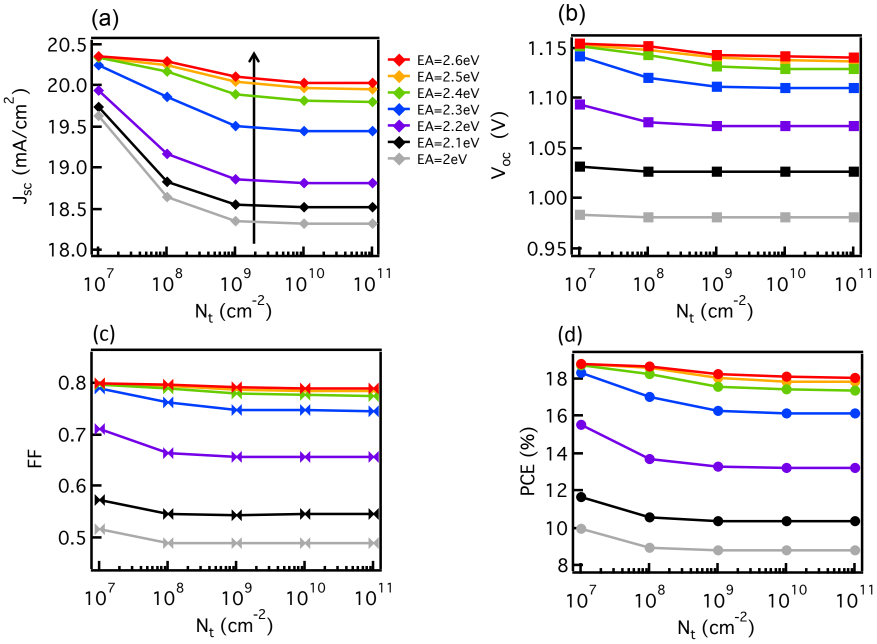

Figure S6 Simulated J_{sc} (a), V_{oc} (b), FF (c), and PCE (d) for devices with different HTL EA: 2.6 eV (red), 2.5 eV (orange), 2.4 eV (green), 2.3 eV (blue), 2.2 eV (purple), 2.1 eV (black), and 2 eV (grey). The arrow indicates the direction of increasing HTL EA.

Referenc:

[1] Q. Lin, Nat. Photonics **9**, 106 (2014).
[2] H.-S. Duan, H. Zhou, Q. Chen, P. Sun, S. Luo, T.-B. Song, B. Bob, and Y. Yang, Phys. Chem. Chem. Phys. **17**, 112 (2014).