Electronic Supplementary Material (ESI) for Energy & Environmental Science.

Supplementary figures

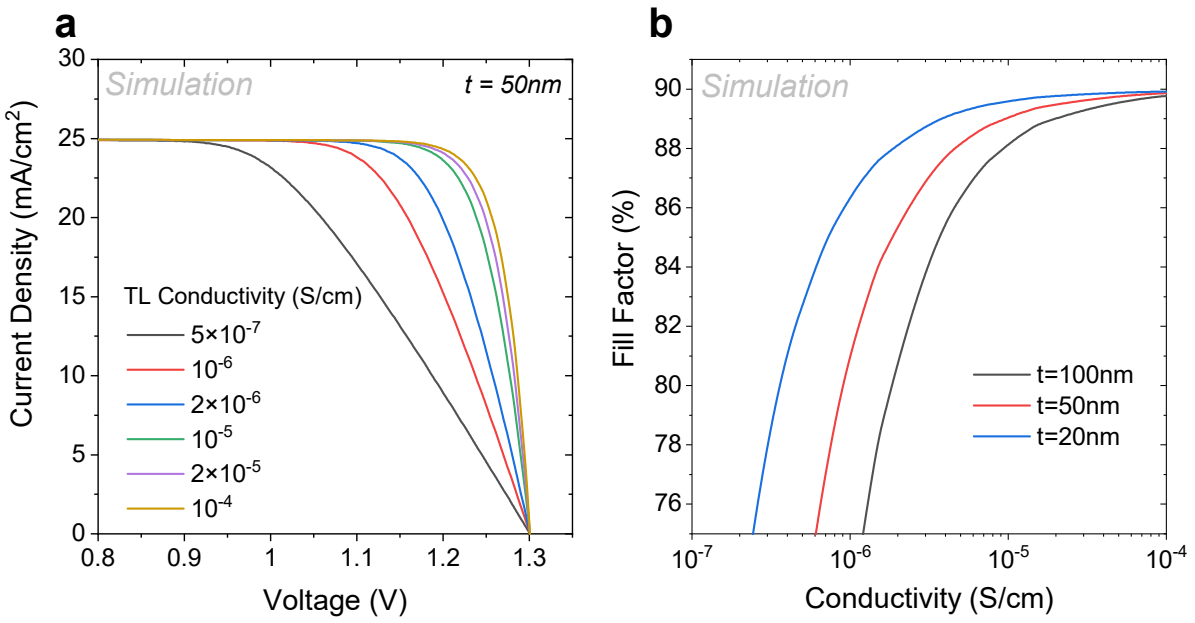

Figure S1: Simulated JV curves (a) as a function of conductivity of a 50 nm-thick transport layer using a one-diode equivalent circuit model where series resistance in the transport layer is the only non-ideal loss. (b) The corresponding maximum achievable fill factor as a function of conductivity.

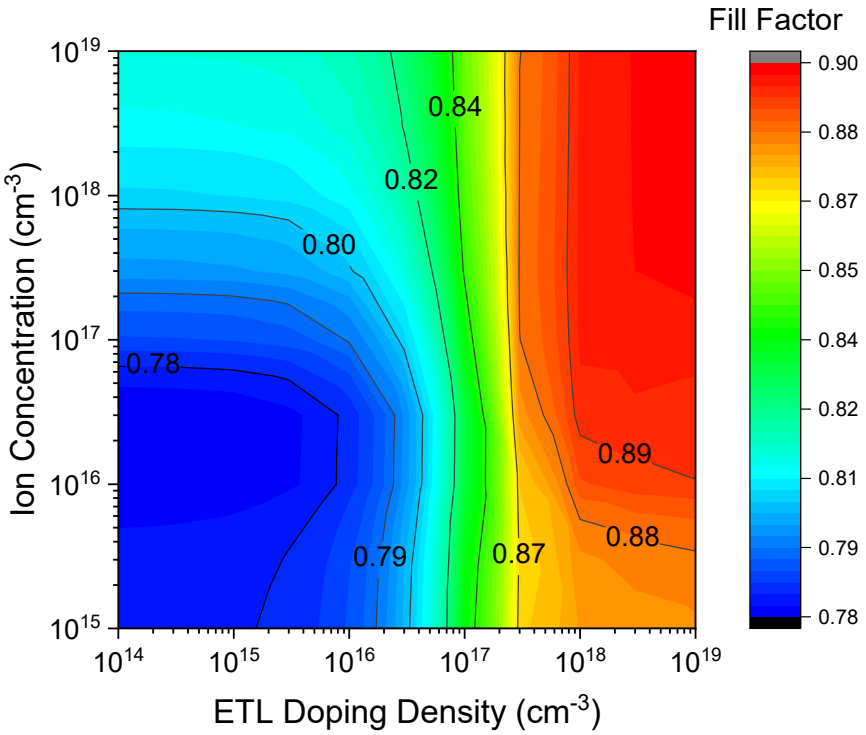

Figure S2: Fill factor as a function of ETL doping density and perovskite ion concentration. Here, $\Delta\phi$= 220 meV and ETL electron mobility = 0.5 cm^2/Vs. Ion concentration has a relatively small influence on achievable FF, relative to the ETL doping density.

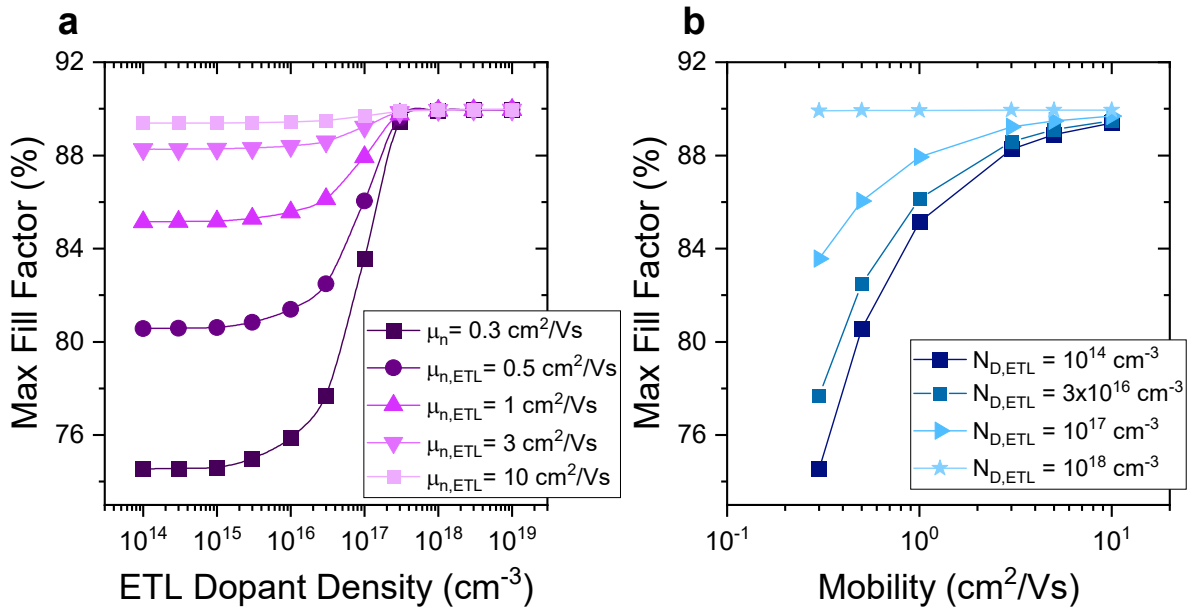

Figure S3: Achievable fill factor simulated via one dimensional equivalent circuit model of figure S1, illustrating influence of ETL electron mobility. In (a) max FF vs ETL dopant density and (b) max FF vs electron mobility.

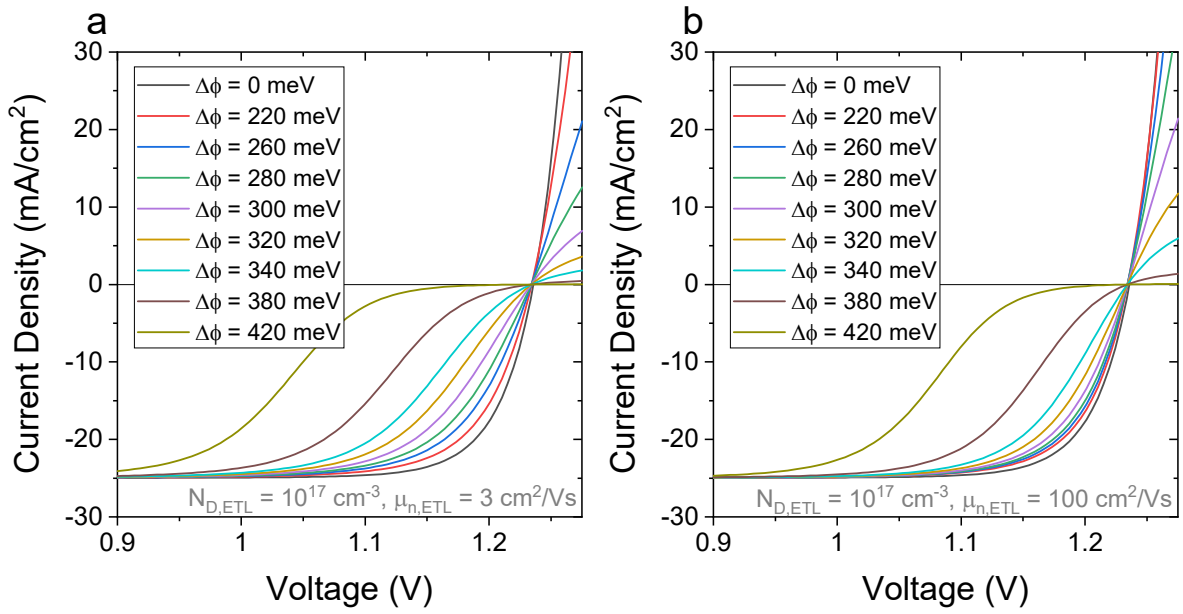

Figure S4: Simulated JV curves as a function of Δϕ for ETL mobility of 3 cm²/Vs (a) and 100 cm²/Vs (b).

Table S1: Fill factor corresponding to JV curves of figure S4.

Δϕ (meV)	Fill Factor, $\mu_{n,ETL}$= 3 cm²/Vs (%)	Fill Factor, $\mu_{n,ETL}$= 100 cm²/Vs (%)
0	88.6	88.6
220	86.1	86.9
260	84.8	86.5
280	83.8	86.2
300	82.6	85.6
320	81.4	84.8
340	80.1	83.8
380	78.0	81.4
420	75.8	78.1

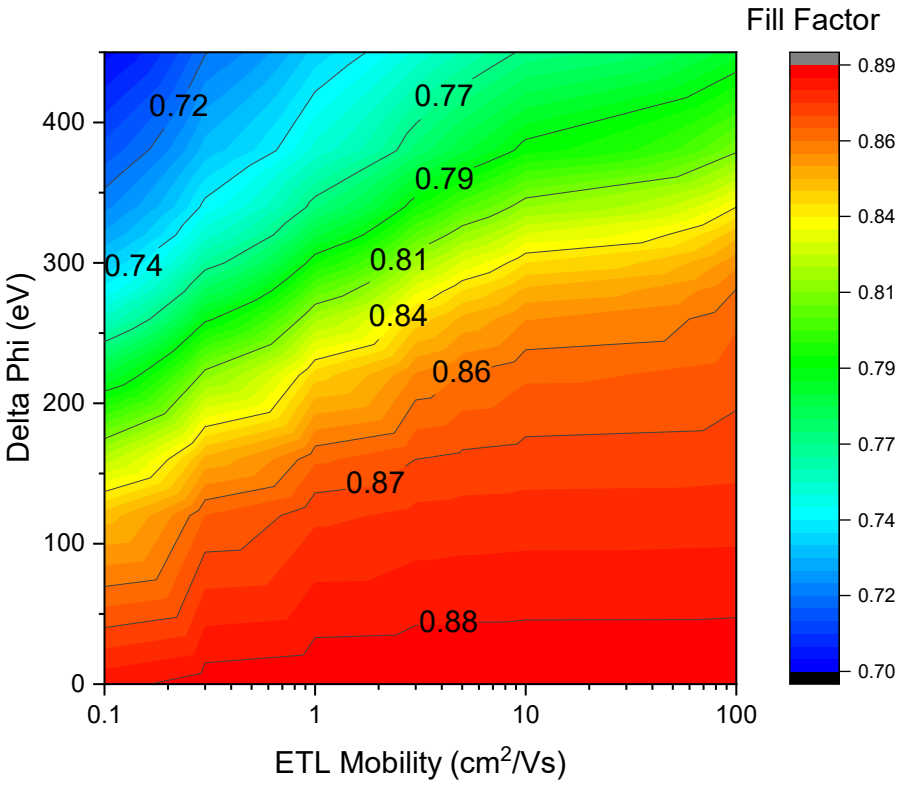

Figure S5: Fill factor as function of ETL mobility and work function difference, Δϕ, where $N_{D,ETL} = 10^{17}$ cm^{-3}.

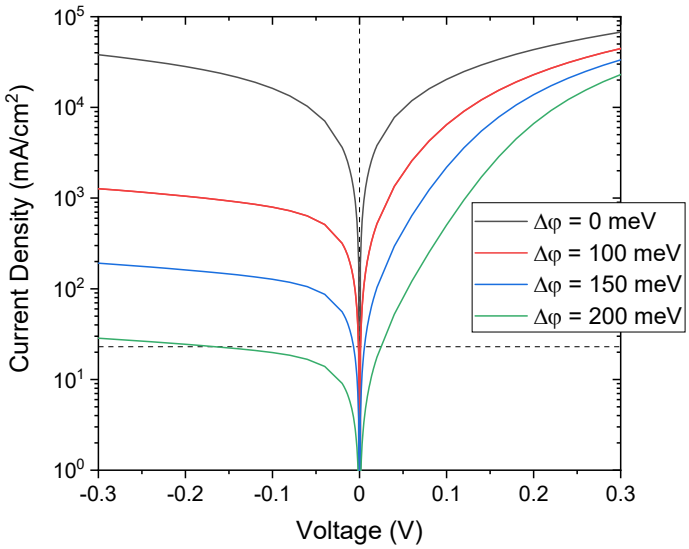

Figure S6: Simulated JV characteristics of an ETL/TCO test structure, illustrating the 'mild' rectification for values of delatphi > 100 meV. The horizontal line marks the approximate maximum power point current for the perovskite solar cells simulated in the main manuscript, illustrating the voltage loss incurred to pass this current.

Simulation parameters

Simulations were performed using COMSOL Multiphysics v5.6. Details of the model can be found in previous publications [1],[2], [3]. Simulation parameters are tabulated below:

Parameter	Value [unit]
Hole Transport Layer	
Relative Permittivity	3
Band Gap	3 [V]
Electron Affinity	2.5 [V]
Effective density of states, valence band	10^{20} [cm^{-3}]
Effective density of states, conduction band	10^{20} [cm^{-3}]
Electron mobility	0.01 [$cm^2/V{\cdot}s$]
Hole mobility	0.1 [$cm^2/V{\cdot}s$]
Dopant defect concentration (p-type)	10^{17} [cm^{-3}]
Thickness	50 [nm]
Electron Transport Layer	
Relative Permittivity	24
Band Gap	3 [V]
Electron Affinity	3.9 [V]
Effective density of states, valence band	10^{20} [cm^{-3}]
Effective density of states, conduction band	10^{20} [cm^{-3}]
Electron mobility	0.5 [$cm^2/V{\cdot}s$]
Hole mobility	0.01 [$cm^2/V{\cdot}s$]
Dopant defect concentration (n-type)	Variable, see text
Thickness	50 [nm]
Perovskite Layer	
Relative Permittivity	64
Band Gap	1.6 [V]
Electron affinity	4.1 [V]
Effective density of states, valence band	10^{19} [cm^{-3}]
Effective density of states, conduction band	10^{19} [cm^{-3}]
Electron mobility	2 [$cm^2/V{\cdot}s$]
Hole mobility	2 [$cm^2/V{\cdot}s$]
Direct recombination coefficient	5.3×10^{-11} [cm^3/s]
Photocurrent density, when illuminated	25 [mA/cm^2]
Thickness	400 [nm]
Cation Concentration	$3x10^{16}$ [cm^{-3}]
Anion Concentration	$3x10^{16}$ [cm^{-3}]
Cation Diffusivity	10^{-8} [cm^2/s]
Anion Diffusivity	10^{-11} [cm^2/s]
TCO Layer	
Relative Permittivity	4
Band Gap	4.0 [V]
Electron affinity	Variable, see text [V]
Effective density of states, valence band	10^{19} [cm^{-3}]
Effective density of states, conduction band	10^{19} [cm^{-3}]
Electron mobility	5 [$cm^2/V{\cdot}s$]
Hole mobility	1 [$cm^2/V{\cdot}s$]
Thickness	130 [nm]
Dopant defect concentration (n-type)	10^{20} [cm^{-3}]

References

[1] D. Walter et al., J. Phys. Chem. C, vol. 122, no. 21, pp. 11270–11281, 2018

[2] J. Peng et al., Science, vol. 371, no. 6527, pp. 390–395, Jan. 2

[3] D. A. Jacobs et al., Journal of Applied Physics. 124, 225702 (2018).