Supplementary Material
To
The effects of interfacial recombination and injection barrier on the electrical characteristics of perovskite solar cells

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A. The computational method used in solving the non-linear Poisson and drift-diffusion equations

In the model, we used the following equations:

$$\frac{\partial^2 V}{\partial x^2} = -\frac{q}{\varepsilon}(p - n - N_A^- + N_D^+) \tag{S1}$$

$$\frac{\partial n}{\partial t} = \frac{\partial}{\partial x}\left(\mu_n n E + D_n \frac{\partial n}{\partial x}\right) + G_n - R_n \tag{S2}$$

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}\left(\mu_p p E - D_p \frac{\partial p}{\partial x}\right) + G_p - R_p \tag{S3}$$

where the physical explanations of all parameters are described in the manuscript. To solve above equations, the Scharfetter-Gummel scheme in the spatial domain and the semi-implicit strategy in the temporal domain are used[1–3]. The one-dimensional discretized forms of Eqs. (S1) - (S3) are respectively given by:

$$\frac{1}{\Delta x^2}\varepsilon_{i+\frac{1}{2}}V_{i+1}^{m+1} - \left[\frac{2}{\Delta x^2}\left(\varepsilon_{i+\frac{1}{2}} + \varepsilon_{i-\frac{1}{2}}\right) + \frac{n_i^m + p_i^m}{V_t}\right]V_i^{m+1} + \frac{1}{\Delta x^2}\varepsilon_{i-\frac{1}{2}}V_{i-1}^{m+1} = -q\left(p_i^m - n_i^m - {N_A}_i^m + {N_D}_i^m\right) - \frac{n_i^m + p_i^m}{V_t}V_i^m \tag{S4}$$

$$\left[\frac{1}{\Delta t} + D_{n,i+\frac{1}{2}}B\left(\frac{V_i^{m+1} - V_{i+1}^{m+1}}{V_t}\right) + D_{n,i-\frac{1}{2}}B\left(\frac{V_i^{m+1} - V_{i-1}^{m+1}}{V_t}\right)\right]n_i^{m+1} - D_{n,i+\frac{1}{2}}B\left(\frac{V_{i+1}^{m+1} - V_i^{m+1}}{V_t}\right)n_{i+1}^{m+1} - D_{n,i-\frac{1}{2}}B\left(\frac{V_{i-1}^{m+1} - V_i^{m+1}}{V_t}\right)n_{i-1}^{m+1} = \frac{1}{\Delta t}n_i^m + G_n^m - R_n(n_i^m, p_i^m) \tag{S5}$$

$$\left[\frac{1}{\Delta t} + D_{p,i+\frac{1}{2}}B\left(-\frac{V_i^{m+1} - V_{i+1}^{m+1}}{V_t}\right) + D_{p,i-\frac{1}{2}}B\left(-\frac{V_i^{m+1} - V_{i-1}^{m+1}}{V_t}\right)\right]p_i^{m+1} - D_{p,i+\frac{1}{2}}B\left(-\frac{V_{i+1}^{m+1} - V_i^{m+1}}{V_t}\right)p_{i+1}^{m+1} - D_{p,i-\frac{1}{2}}B\left(-\frac{V_{i-1}^{m+1} - V_i^{m+1}}{V_t}\right)p_{i-1}^{m+1} = \frac{1}{\Delta t}p_i^m + G_n^m - R_n(n_i^m, p_i^m) \tag{S6}$$

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where the superscript m and subscript i indicate the discretized temporal and spatial steps, respectively. $V_t = \frac{k_B T}{q}$ is the thermal voltage and $B(x) = \frac{x}{e^x - 1}$ is the Bernauli's function.

The grid spacing is 1 nm. The convergence condition for the steady solution calculation is given by $\left|\frac{J^{m+1} - J^m}{J^m}\right| < 10^{-10}$.

B. The charge carrier generation profile throughout the device

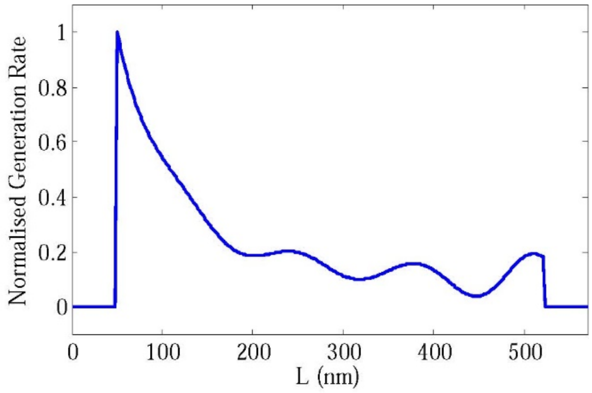

FIG. S1. Normalized generation rate of charge carriers throughout the device.

C. Additional simulation results

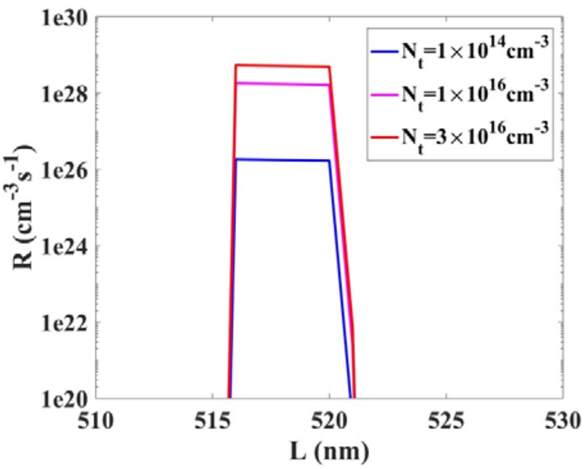

FIG. S2. The interfacial recombination rate profiles of PSCs with trap density from1×10^{14} to $3 \times 10^{16} cm^{-3}$ in the bottom interfacial recombination region.

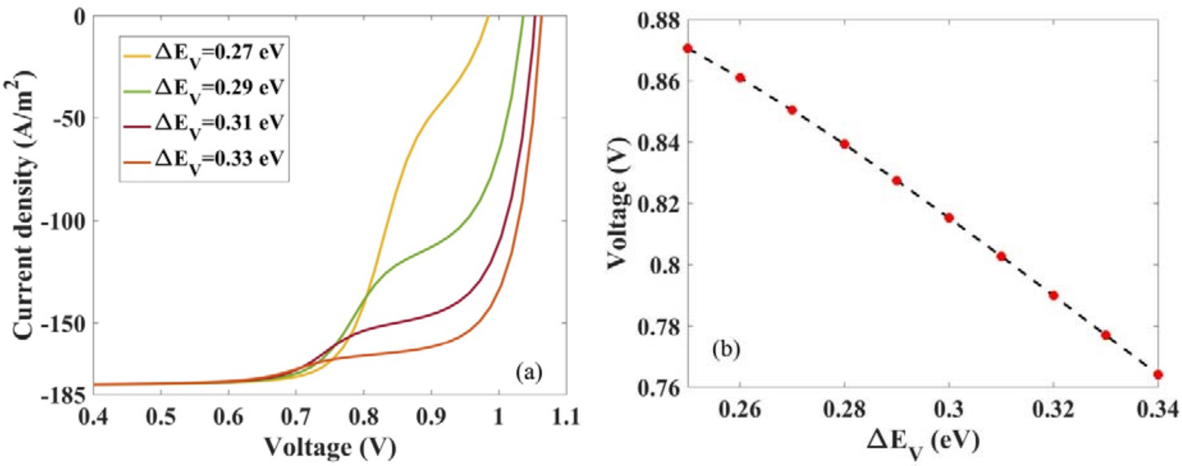

FIG. S3. The effect of the hole injection barrier between the perovskite layer and HTL on the applied voltage forming the zero electric field at the interface. (a) *J-V* characteristics of PSCs with various hole injection barrier. The trap density at the bottom interface is $3 \times 10^{16} cm^{-3}$. (b) The applied voltage corresponding to the zero electric field dependence of the hole injection barrier.

References

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