Supplementary Information for "How much physics is in a current-voltage curve? Inferring defect properties from photovoltaic device measurements"

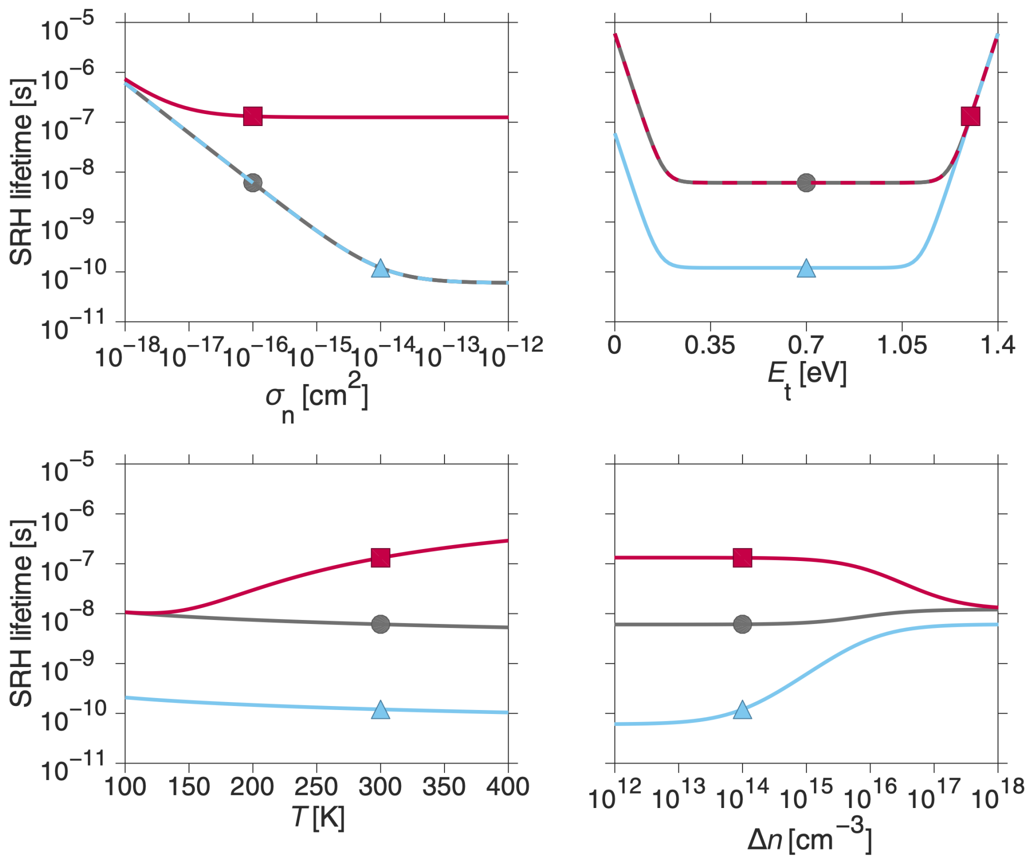

Figure S1: SRH lifetime sensitivity plots showing a baseline calculation (grey dot) along with variations in σ_n (blue) and E_t (red), also showing dependence on illumination (injection level Δn) and temperature.

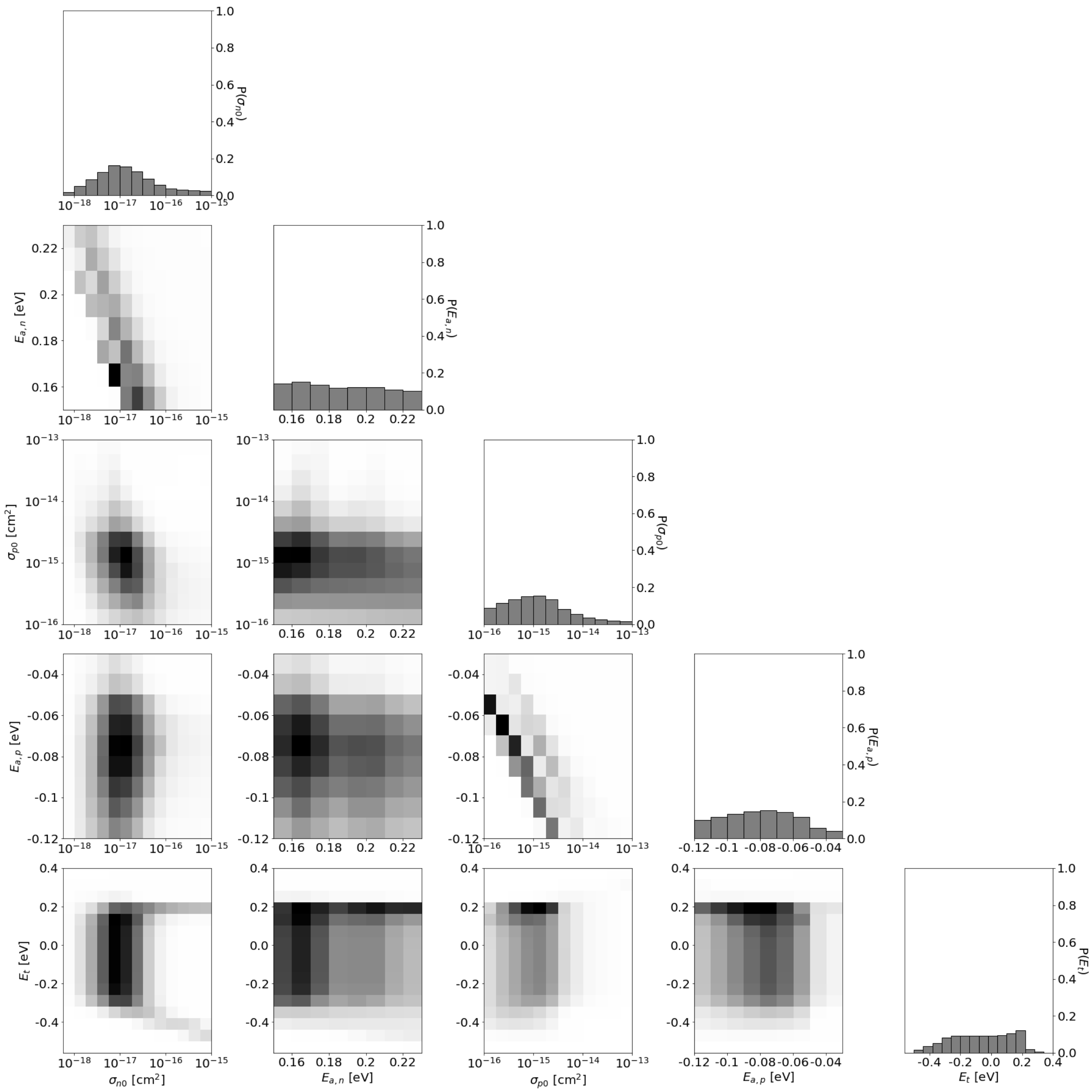

Figure S2: Full five-parameter probability distribution.

<table>
<tr><th>parameter name</th><th>value / setting</th><th>Ref.</th><th>notes</th></tr>
<tr><td>Device Area</td><td>3.55 cm^2</td><td>measured 4.00 cm^2; Ref. 1</td><td>adjusted downward from 4.00 cm^2 due to boundary effects (i.e., 1-Sun J_{SC} of real cell does not match QE-calculated J_{SC}). Partially because aperture is used during measurement.)</td></tr>
<tr><td>Surface texture</td><td>No surface texturing</td><td></td><td></td></tr>
<tr><td>Surface charge</td><td>No surface charge</td><td>2</td><td>Ref. 2 lists no surface charge for the conventional cell. A rear surface charge of 10^{10} cm^{-2} didn't seem to matter much, either. Also see PC1Dmod 6-2 manual, p. 13.</td></tr>
<tr><td>Reflectance: Front External</td><td>Coated; broadband reflectance = 0.69%; inner layer (thickness, index) = (76 nm, 1.98)</td><td>1</td><td>Used high end of thickness, 73±3 nm, to better fit reflectance data measured experimentally</td></tr>
<tr><td>Reflectance: Rear External</td><td>Fixed (0%)</td><td></td><td></td></tr>
<tr><td>Reflectance: Internal Reflectance</td><td>Front surface: specular, 30% (first bounce and subsequent bounces); Rear surface: specular, 95% (first bounce and subsequent bounces);</td><td></td><td>Adjusted to fit experimentally measured reflectance</td></tr>
<tr><td>Contact definition</td><td><table>
<tr><th></th><th>internal series resistance</th><th>distance from surface</th></tr>
<tr><td>emitter</td><td>$10^{-8}\Omega$</td><td>0 μm</td></tr>
<tr><td>base</td><td>0.18 Ω</td><td>400 μm</td></tr>
</table></td><td>base and emitter thickness: Ref. 1</td><td></td></tr>
<tr><td>Internal shunt element 1</td><td>conductor, 5.83×10^{-4}, anode/cathode/ideality = 400/0/1</td><td></td><td>Fitted to experimental J–V data</td></tr>
<tr><td>Global band structure</td><td>electron affinity: 4.05 eV</td><td></td><td>Other parameters defined by configuration file.</td></tr>
</table>

Table S1: PC1D **device** parameters for simulating $JVTi$ data.

parameter name	**value / setting**	**Ref.**	**notes**
Thickness	400 μm	1	
Dielectric constant	11.7		
Optical properties: Refractive index–External	data file	3	
Optical properties: Intrinsic absorption – External absorption coeff.	data file	3	
Optical properties: Free-carrier absorption	Enabled; $\alpha = 2.85 \times 10^{-26} n\lambda^{2.6} + 1.64 \times 10^{-25} p\lambda^{2.4}$	4	
Background doping	p-type; $4.979{\times}10^{15}$ cm^{-3}; resistivity = 2.85 Ω-cm	1	
First front diffusion	Enabled, n-type; calculated from Erfc, sheet resistance = 27.01, junction depth = 1.3 μm (peak doping / depth factor / and peak position = 1.062e20, 0.4516, 0)		Calculated in-program. Iterated the sheet resistance and depth factor to match the experimental QE.
Second front diffusion	No second front diffusion		
First/second rear diffusion	No rear diffusion		
Bulk recombination	fitting parameter		
Front surface	$1{\times}10^7$ cm/s, $E_t = E_i$	suggested from Ref. 2	
Rear surface	$1{\times}10^7$ cm/s, $E_t = E_i$	suggested from Ref. 2	

Table S2: PC1D **material** parameters for simulating $JVTi$ data.

parameter name	**value / setting**	**notes**
Excitation mode	Transient, number of time steps = 100; time step size = 1 s; time step at t=0 = 1e-09	
Temperature	*input parameter*	
Base circuit	Source: 0 Ω-cm^2 resistance; sweep from -0.5 to $+1.0$ V	zero resistance necessary for voltage to sweep full range (vs. some subset)
Collector circuit	all parameters set to zero	
Primary illumination – intensity	Enable; Front; level is input parameter; AM1.5G spectrum	
Secondary illumination	disabled	

Table S3: PC1D **excitation** parameters for simulating $JVTi$ data.

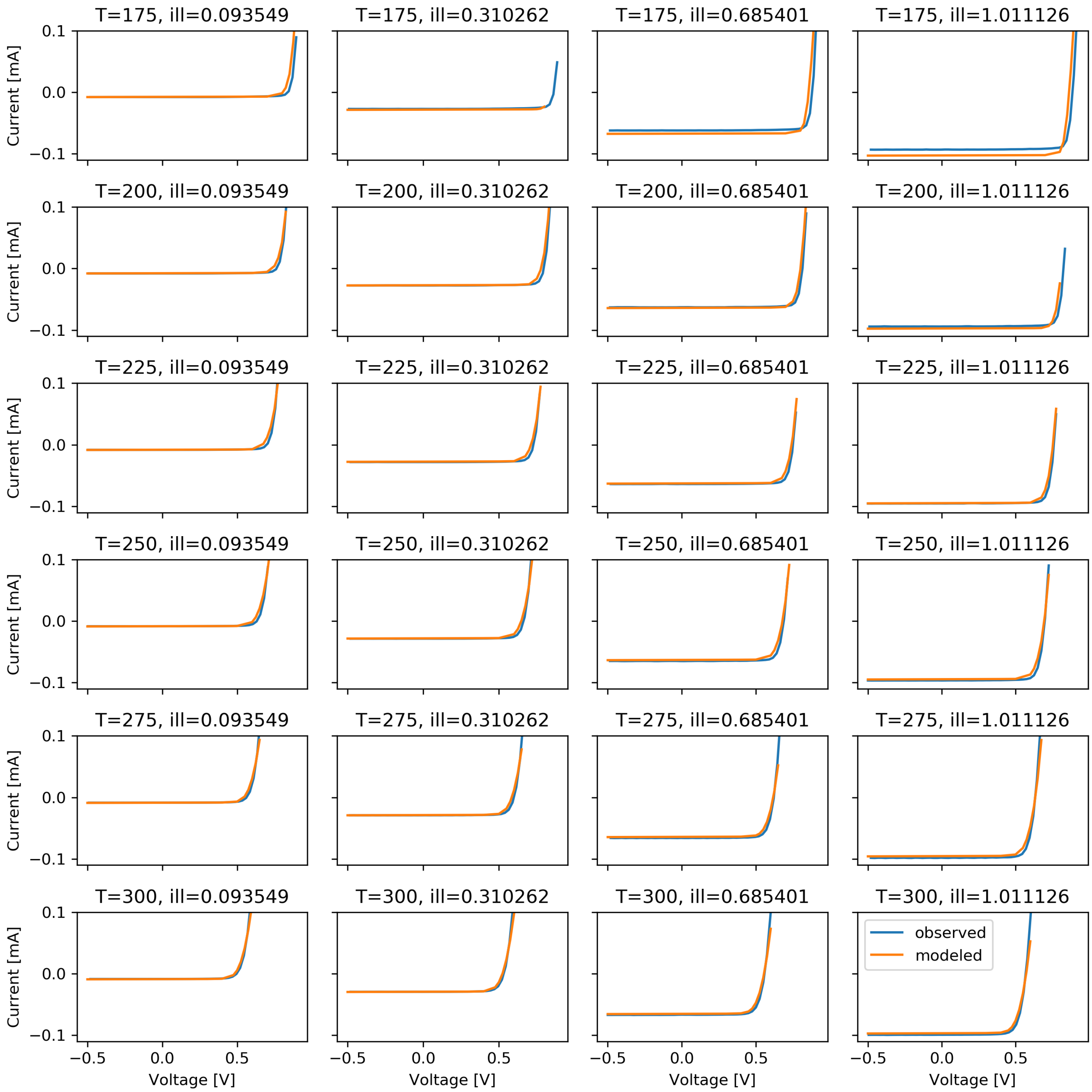

Figure S3: Comparison between modeled and simulated (for highest-probability set of Arrhenius parameters) at every experimental condition (illumination levels in Suns, temperatures in K). Lack of high-voltage data for some conditions was due to numerical convergence errors.

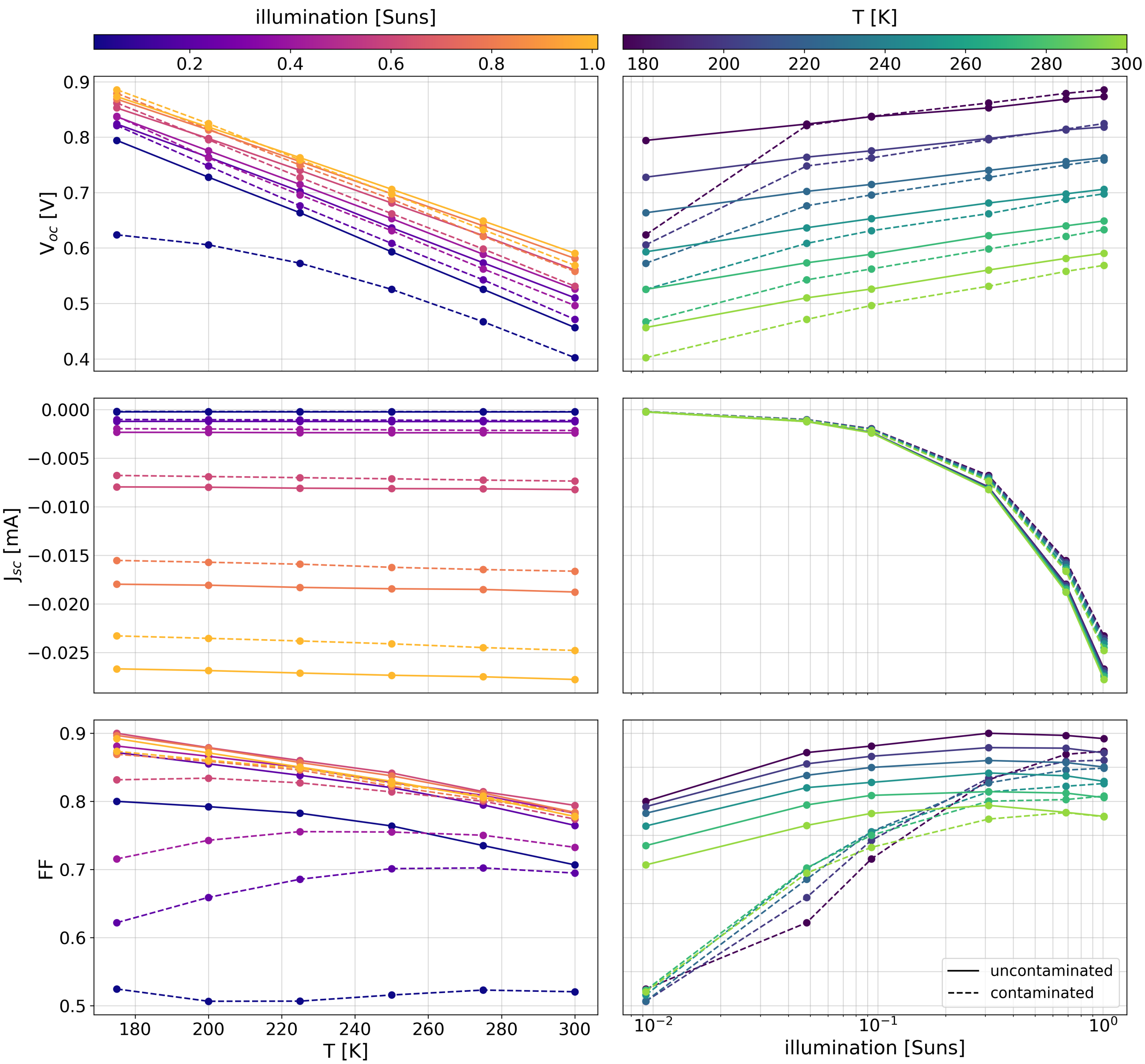

Figure S4: Open-circuit voltage (V_{oc}), short-circuit current (J_{sc}), and fill factor (FF) for contaminated (dotted line) and uncontaminated (solid line) samples plotted against temperature and illumination intensity, with values of other experimental condition in each case indicated by the colorbars.

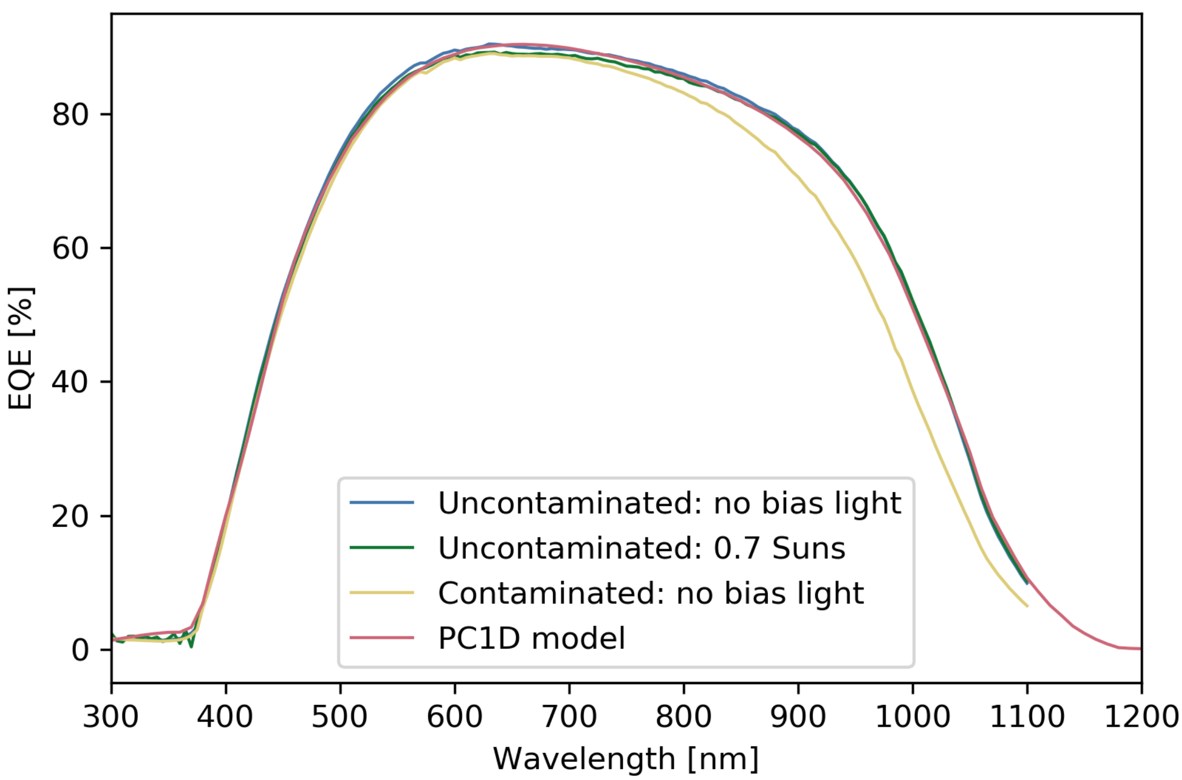

Figure S5: External quantum efficiency data with and without bias light for the uncontaminated sample, without bias light for contaminated sample, and PC1D model output for unbiased QE with parameters calibrated on uncontaminated sample.

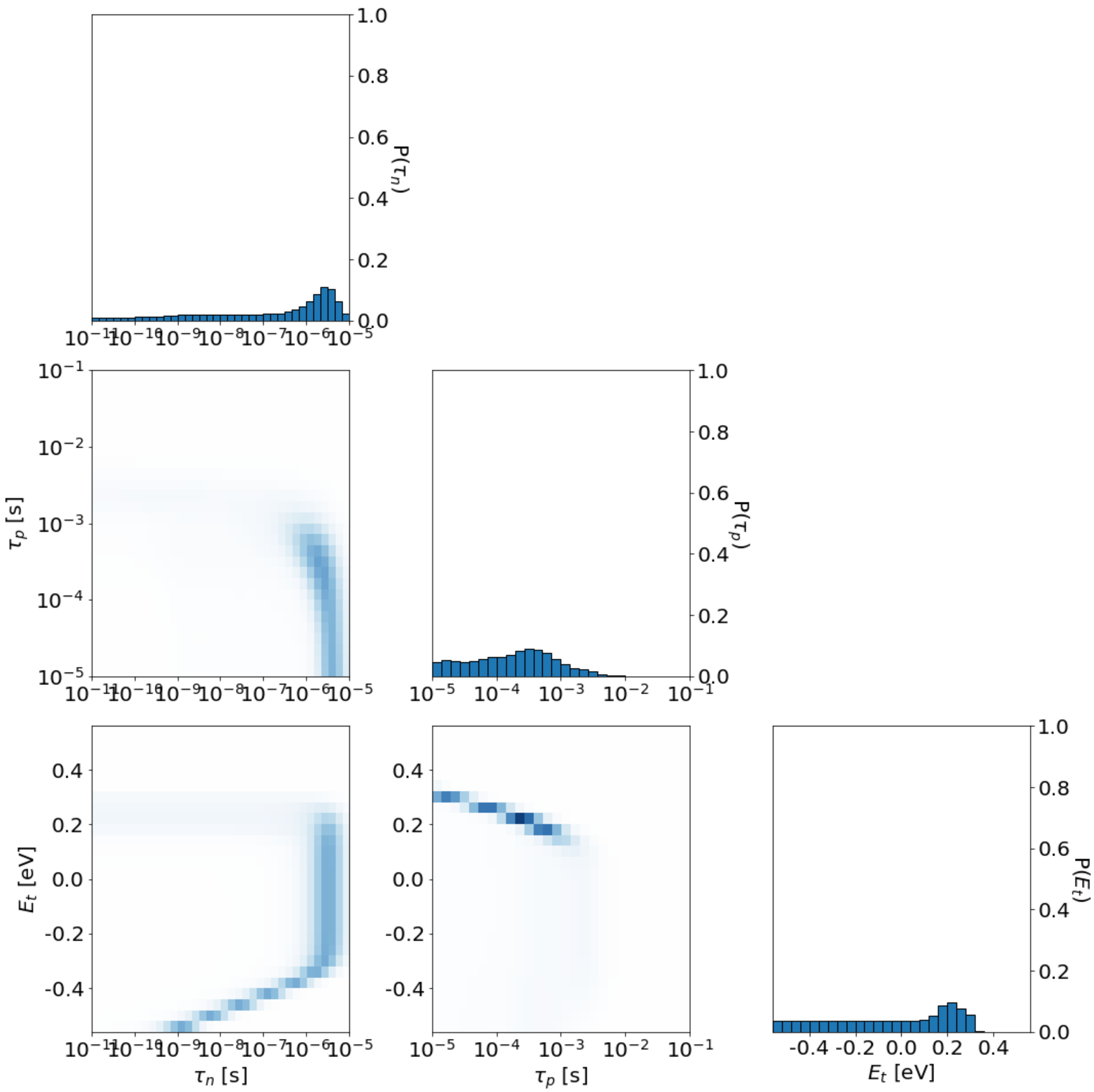

Figure S6: Results for the three-parameter fit at 300K using data only at 1 Sun light intensity.

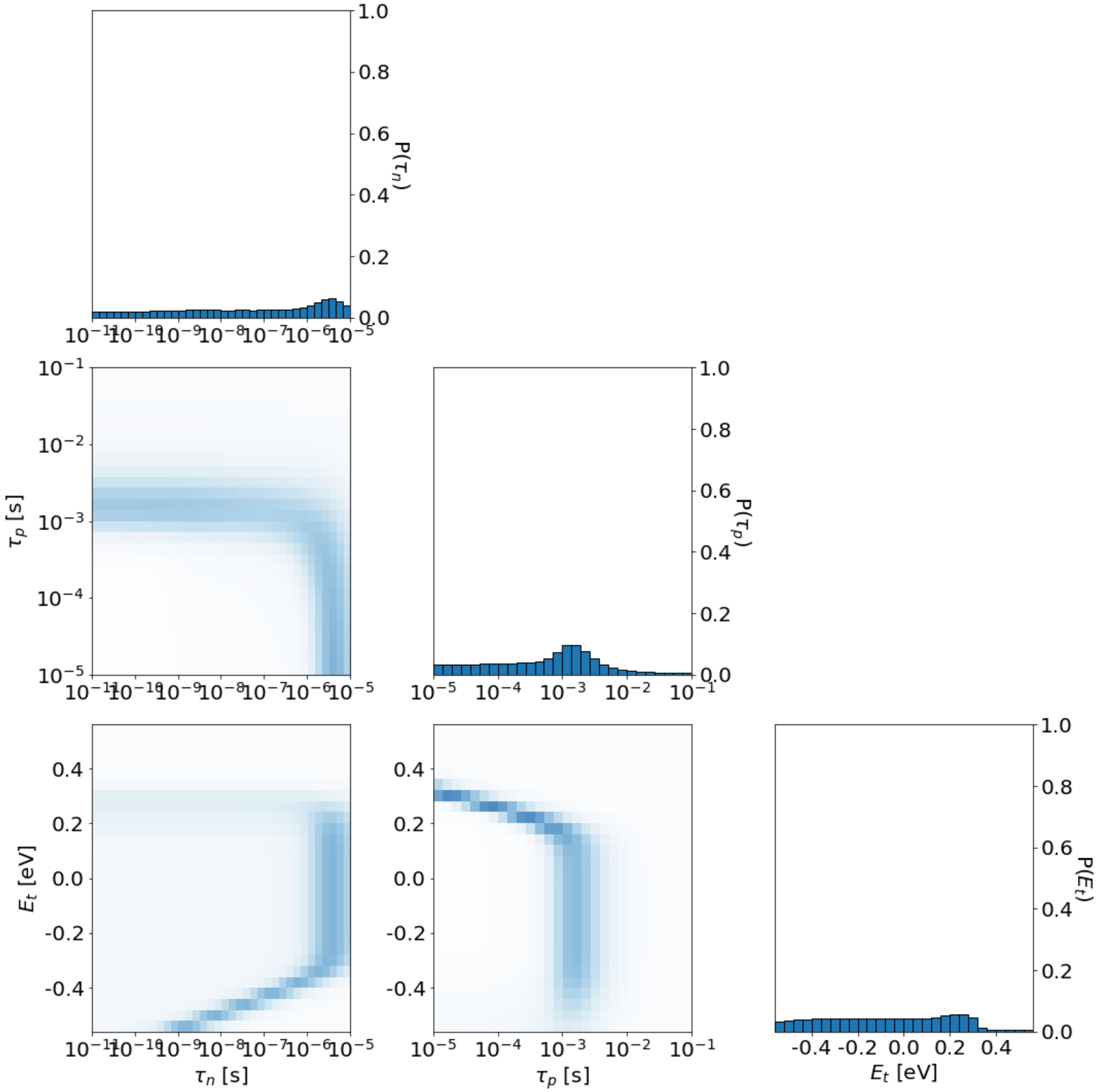

Figure S7: Results for the three-parameter fit at 300K using data only at V_{oc} for each JV curve.

References

[1] V. Vähänissi, A. Haarahiltunen, H. Talvitie, M. Yli-koski, and H. Savin, "Impact of phosphorus gettering parameters and initial iron level on silicon solar cell properties," *Progress in Photovoltaics: Reseach and Applications*, pp. 1127–1135, 2013.

[2] A. Fell, K. R. McIntosh, P. P. Altermatt, G. J. M. Janssen, R. Stangl, A. Ho-Baillie, H. Steinkemper, J. Greulich, M. Müller, B. Min, K. C. Fong, M. Hermle, I. G. Romijn, and M. D. Abbott, "Input parameters for the simulation of silicon solar cells in 2014," *IEEE Journal of Photovoltaics*, vol. 5, no. 4, pp. 1250–1263, July 2015.

[3] M. A. Green, "Self-consistent optical parameters of intrinsic silicon at 300k including temperature coefficients," *Solar Energy Materials and Solar Cells*, vol. 92, no. 11, pp. 1305 – 1310, 2008. [Online]. Available: http://www.sciencedirect.com/science/article/pii/S0927024808002158

[4] M. Rüdiger, J. Greulich, A. Richter, and M. Hermle, "Parameterization of free carrier absorption in highly doped silicon for solar cells," *IEEE Transactions on Electron Devices*, vol. 60, no. 7, pp. 2156–2163, July 2013.