Supporting Information for "IonMonger: a free and fast planar perovskite solar cell simulator with coupled ion vacancy and charge carrier dynamics"

N. E. Courtier[1,*], J. M. Cave[2], A. B. Walker[2], G. Richardson[1], and J. M. Foster[3]
[1]Mathematical Sciences, University of Southampton, Southampton, UK
[2]Department of Physics, University of Bath, Bath, UK
[3]School of Mathematics and Physics, University of Portsmouth, Portsmouth, UK
*Corresponding author: N.E.Courtier@soton.ac.uk

This document contains five tables which contain: 1) the model variables, 2) the computational settings, 3) the dimensional input parameters, 4) the computed properties, and 5) the dimensionless parameters for the `IonMonger` code. This code is freely available (under an AGPL-3.0 copyleft license) on GitHub at `https://github.com/PerovskiteSCModelling/IonMonger`.

Table 1: Table of model variables.

Symbol	Description	Unit
$n(x,t)$	Electron concentration	m^{-3}
$p(x,t)$	Hole concentration	m^{-3}
$P(x,t)$	Iodide ion vacancy density	m^{-3}
$\phi(x,t)$	Electric potential	V
$j^n(x,t)$	Electron current density	Am^{-2}
$j^p(x,t)$	Hole current density	Am^{-2}
$F^P(x,t)$	Iodide ion vacancy flux	$\mathrm{m}^2\mathrm{s}^{-1}$
$E(x,t)$	Electric field	Vm^{-1}
$V(t)$	Applied voltage	V
$J(t)$	Total current density	mAcm^{-2}

Table 2: Table of computational settings.

Symbol	Description
N	Number of subintervals, with $N+1$ as the number of grid points
`rtol`	Relative temporal tolerance for `ode15s` solver
`atol`	Absolute temporal tolerance for `ode15s` solver

[1]Note that the effective doping densities (d_E and d_H) should be chosen to be less than 20 times smaller than the effective DoS in each transport layer (g_c^E and g_c^H, respectively) for compatibility with the use of the Boltzmann approximation in the model.

Table 3: Table of input parameters, in which the abbreviation DoS denotes the density of states.

Symbol	Description	Unit
ε_0	Permittivity of free space	Fm^{-1}
q	Elementary charge	C
F_{ph}	Incident photon flux at 1 Sun	$\mathrm{m}^{-2}\mathrm{s}^{-1}$
k_B	Boltzmann constant	eVK^{-1}
T	Temperature	K
I_s	Intensity of incident light	Suns
	Perovskite Properties	
α	Absorption coefficient	m^{-1}
b	Width	nm
ε_A	Permittivity	ε_0
D_n	Electron diffusion coefficient	$\mathrm{m}^2\mathrm{s}^{-1}$
D_p	Hole diffusion coefficient	$\mathrm{m}^2\mathrm{s}^{-1}$
E_C	Conduction band minimum	eV
E_V	Valence band maximum	eV
g_c	Conduction band DoS	m^{-3}
g_v	Valence band DoS	m^{-3}
D_I	Iodide ion vacancy diffusion coefficient	$\mathrm{m}^2\mathrm{s}^{-1}$
$\hat{N}_0$	Mean density of ion vacancies	m^{-3}
β	Bimolecular rate constant	$\mathrm{m}^3\mathrm{s}^{-1}$
τ_n	Electron SRH pseudo-lifetime	s
τ_p	Hole SRH pseudo-lifetime	s
	Interface Properties	
$\beta^{E,H}$	Bimolecular rate constant for interface indicated by superscript	$\mathrm{m}^3\mathrm{s}^{-1}$
$\nu_n^{E,H}$	Electron recombination velocity towards interface indicated by superscript	ms^{-1}
$\nu_p^{E,H}$	Hole recombination velocity towards interface indicated by superscript	ms^{-1}
	ETL Properties	
b_E	Width	nm
d_E	Effective doping density[1]	m^{-3}
D_E	Electron diffusion coefficient	$\mathrm{m}^2\mathrm{s}^{-1}$
ε_E	Permittivity	ε_0
E_c^E	Conduction band maximum	eV
g_c^E	Effective conduction band DoS	m^{-3}
	HTL Properties	
b_H	Width	nm
d_H	Effective doping density[1]	m^{-3}
D_H	Hole diffusion coefficient	$\mathrm{m}^2\mathrm{s}^{-1}$
ε_H	Permittivity	ε_0
E_v^H	Valence band minimum	eV
g_v^H	Effective valence band DoS	m^{-3}

Table 4: Table of computed properties.

Symbol	Description	Unit
E_{f_E}	Fermi level in the ETL	eV
E_{f_H}	Fermi level in the HTL	eV
L_D	Perovskite Debye length	nm
$G(x,t)$	Photo-generation rate	$\mathrm{m}^{-3}\mathrm{s}^{-1}$
G_0	Typical generation rate	$\mathrm{m}^{-3}\mathrm{s}^{-1}$
n_0	Typical electron concentration in perovskite ($k_E d_E$)	m^{-3}
p_0	Typical hole concentration in perovskite ($k_H d_H$)	m^{-3}
$R(x,t)$	Bulk recombination rate	$\mathrm{m}^{-3}\mathrm{s}^{-1}$
$\bar{R}_l(t)$	ETL/perovskite interface recombination flux	$\mathrm{m}^{-2}\mathrm{s}^{-1}$
$\bar{R}_r(t)$	Perovskite/HTL interface recombination flux	$\mathrm{m}^{-2}\mathrm{s}^{-1}$
τ_{ion}	Characteristic timescale	s
V_{bi}	Built-in voltage	V
V_T	Thermal voltage	mV

Table 5: Table of dimensionless parameters.

Symbol	Definition	Description
δ	$d_E/\hat{N}_0$	Ratio between the ETL doping and the ion vacancy densities
χ	d_H/d_E	Ratio between the HTL and ETL doping densities
σ	$d_E/(G_0\tau_{ion})$	Characteristic ratio between the timescales of electronic and ionic motion
κ_p	$D_p d_H/(G_0 b^2)$	Dimensionless hole diffusion coefficient in perovskite
κ_n	$D_n d_E/(G_0 b^2)$	Dimensionless electron diffusion coefficient in perovskite
κ_E	$D_E\kappa_n/D_n$	Dimensionless electron diffusion coefficient in ETL
κ_H	$D_H\kappa_p/D_p$	Dimensionless hole diffusion coefficient in HTL
λ	L_D/b	Dimensionless (ionic) Debye length in perovskite
λ_E	$\sqrt{\frac{\varepsilon_E\hat{N}_0}{\varepsilon_A d_E}}\lambda$	Dimensionless Debye length in ETL
λ_H	$\sqrt{\frac{\varepsilon_H\hat{N}_0}{\varepsilon_A d_H}}\lambda$	Dimensionless Debye length in HTL
Φ	V/V_T	Dimensionless applied voltage
Φ_{bi}	V_{bi}/V_T	Dimensionless built-in voltage
r_E	$\varepsilon_E/\varepsilon_A$	Ratio between the ETL and perovskite permittivities
r_H	$\varepsilon_H/\varepsilon_A$	Ratio between the HTL and perovskite permittivities
w_E	b_E/b	Dimensionless ETL width
w_H	b_H/b	Dimensionless HTL width