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Supplementary information for 'IonMonger 2.0: Software for free, fast and versatile simulation of current, voltage and impedance response of planar perovskite solar cells'

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1 Tables of symbol definitions

This section 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.

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 $N+1$
`rtol`	Relative temporal tolerance for `ode15s` solver
`atol`	Absolute temporal tolerance for `ode15s` solver
ϕ_{disp}	Dimensionless electric potential offset

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 effective DoS	m^{-3}
g_v	Valence band effective 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 (interface indicated by superscript)	
$\beta^{E,H}$	Bimolecular rate constant	$\mathrm{m}^3\mathrm{s}^{-1}$
$\nu_n^{E,H}$	Electron recombination velocity towards interface	ms^{-1}
$\nu_p^{E,H}$	Hole recombination velocity towards interface	ms^{-1}
	ETL Properties	
b_E	Width	nm
d_E	Effective doping density	m^{-3}
D_E	Electron diffusion coefficient	$\mathrm{m}^2\mathrm{s}^{-1}$
ε_E	Permittivity	ε_0
E_c^E	Conduction band reference energy	eV
g_c^E	Conduction band effective DoS	m^{-3}
	HTL Properties	
b_H	Width	nm
d_H	Effective doping density	m^{-3}
D_H	Hole diffusion coefficient	$\mathrm{m}^2\mathrm{s}^{-1}$
ε_H	Permittivity	ε_0
E_v^H	Valence band reference energy	eV
g_v^H	Valence band effective DoS	m^{-3}

Table 4 Table of optional input parameters supported with v2.0. If these parameters are omitted, they will be set to their default values.

Symbol	Description	Default value	Unit
$\mathcal{S}_E$	ETL statistical integral	exp	dimensionless
$\mathcal{S}_H$	HTL statistical integral	exp	dimensionless
E_{ct}	Cathode workfunction	E_f^E	eV
E_{an}	Anode workfunction	E_f^H	eV
A_n	Electron-dominated Auger recombination rate	0	$\mathrm{m}^6\mathrm{s}^{-1}$
A_p	Hole-dominated Auger recombination rate	0	$\mathrm{m}^6\mathrm{s}^{-1}$
R_s	External series resistance	0	Ω
R_p	Shunt/parallel resistance	Inf	Ω
A	Cell area	1	cm^2
$E_f^E = -W_E$	ETL work function (overrides d_E)	$E_c^E + V_T\mathcal{S}_E^{-1}\left(d_E/g_c^E\right)$	eV
$E_f^H = -W_H$	HTL work function (overrides d_H)	$E_v^H - V_T\mathcal{S}_H^{-1}\left(d_H/g_v^H\right)$	eV

Table 5 Table of computed properties.

Symbol	Description	Unit
E_{f_E} (or d_E)	Fermi level in the ETL (or ETL effective doping density)	eV (or m^{-3})
E_{f_H} (or d_H)	Fermi level in the HTL (or HTL effective doping density)	eV (or m^{-3})
L_D	Perovskite Debye length	nm
$G(x,t)$	Photo-generation rate	$\mathrm{m}^{-3}\mathrm{s}^{-1}$
G_0	Typical generation rate	$\mathrm{m}^{-3}\mathrm{s}^{-1}$
k_E	Typical electron ratio across ETL interface	-
k_H	Typical hole ratio across HTL interface	-
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	$\mathrm{m}^{-3}\mathrm{s}^{-1}$
$R_l(t)$	ETL/perovskite interface recombination flux	$\mathrm{m}^{-2}\mathrm{s}^{-1}$
$R_r(t)$	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	V

2 Typical parameter values for a TiO_2/MAPI/spiro-MeOTAD cell

Symbol	Name	Values	Unit	Ref.
T	Temperature	298	K	
-	Light entering through	ETL	-	
Perovskite (MAPI)				
b	Perovskite width	400	nm	
ε_p	Permittivity	24.1	ε_0	[1]
α	Absorption coefficient	1.3×10^7	m^{-1}	[6]
g_c	Conduction band effective DoS	8.1×10^{24}	m^{-3}	[1]
g_v	Valence band effective DoS	5.8×10^{24}	m^{-3}	[1]
E_c	Conduction band edge	-3.7	eV	[10]
E_v	Valence band edge	-5.4	eV	[10]
D_n	Electron diffusivity	1.7×10^{-4}	m^2s^{-1}	[11]
D_p	Hole diffusivity	1.7×10^{-4}	m^2s^{-1}	[11]
N_0	Mean anion vacancy density	1.6×10^{25}	m^{-3}	[4]
D_P	Anion vacancy diffusivity	1×10^{-17}	m^2s^{-1}	
ETL (TiO_2)				
g_c^E	Conduction band effective DoS	2×10^{23}	m^{-3}	[7]
d_E	Effective doping density	2×10^{22}	m^{-3}	
D_E	Electron diffusivity	1.3×10^{-5}	m^2s^{-1}	[12]
ε_E	Permittivity	10	ε_0	
b_E	ETL width	100	nm	
E_c^E	Conduction band edge	-4.13	eV	[2]
HTL (spiro-MeOTAD)				
g_v^H	Valence band effective DoS	1×10^{26}	m^{-3}	[8]
d_H	Effective doping density	1×10^{25}	eV	
D_H	Hole diffusivity	1×10^{-6}	m^2s^{-1}	[12]
ε_H	Permittivity	3	ε_0	
b_H	HTL width	200	nm	
E_v^H	Valence band edge	-5.1	eV	[3]

Table 6 Material parameters representative of a typical TiO_2/MAPI/spiro-MeOTAD cell with standard architecture. When non-Boltzmann statistics are used, the TiO_2 is assumed to have parabolic bands and the spiro-MeOTAD is assumed to have Gaussian bands with width $s = 3.73$ [5,9,13].

Symbol	Name	Values	Unit
Perovskite bulk			
β	Bi-molecular rate constant	1.5×10^{-14}	m^3s^{-1}
τ_p	Hole SRH psuedo-lifetime	3×10^{-7}	s
τ_n	Electron SRH psuedo-lifetime	3×10^{-7}	s
A_n	Electron Auger coefficient	0	m^6s^{-1}
A_p	Hole Auger coefficient	0	m^6s^{-1}
ETL/perovskite interface			
ν_p^E	Hole recombination velocity	10	ms^{-1}
ν_n^E	Electron recombination velocity	10^5	ms^{-1}
β_E	Bi-molecular rate constant	0	m^4s^{-1}
HTL/perovskite interface			
ν_p^H	Hole recombination velocity	10^5	ms^{-1}
ν_n^H	Electron recombination velocity	0.1	ms^{-1}
β_H	Bi-molecular rate constant	0	m^4s^{-1}

Table 7 Recombination parameters for a typical TiO_2/MAPI/spiro-MeOTAD cell.

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