User Manual

This documents describes the necessary input files and the various options available in this software. The manual will be updated with more detailed instructions when I have time, but feel free to contact me if you have any questions!

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Settings.ini

This file contains all material, experiment and numerical parameters necessary to run the simulation. Some parameters are mandatory and must be listed and given a value while others are optional and are assigned a default value if left out. Some features are currently being developed and might be mandatory even though these have no actual effect on the simulation. Make sure that the parameters are entered under the correct section and without typos, otherwise the program may crash without warning. All values should be given in SI units, powers of ten can be specified using the notation xEy, where x and y are defined by $x \cdot 10^y$.

[general]

The simulation calculates values for charge carrier concentrations and the electric potential for each point in a lattice with chosen dimensions.

points_x - The number of lattice points in the x-direction. Integer; mandatory.

points_y - The number of lattice points in the y-direction. Integer; optional, default value "1".

length_x - The length of the lattice in the x-direction. Decimal number; mandatory.

length_y - The length of the lattice in the y-direction. Decimal number; optional, default value length_x.

Two separate files containing the morphology of the materials in the simulated system and the dopant concentrations (the dopant file is being phased out) are also needed to run the program.

morphology_file - The name of the file containing the morphology of the simulated system, including file extension. Text string. Mandatory.

dopants_file - The name of the file containing the doping concentration, including file extension. Text string; optional, if this file is left out, the simulation assumes that there are no dopants.

output_full_data - Chose if you want the program to output the raw data files, containing the calculated charge carrier concentrations and potential as functions of x and y, as well as derived parameters, such as the electron and hole currents. Boolean; optional, default value true.

So far, only a constant generation rate has been implemented and generation can be set to occur either within the bulk of a material or at both sides of an interface. The latter is meant to be used in organic donor/acceptor solar cells and requires one of the materials to have a higher HOMO level and the other to have lower LUMO level. Recombination can occur within a material, across an interface or via mid-gap states. The different modes can be turned on or off.

recombination_mode_0 - Recombination between holes and electrons in the bulk of materials. Boolean; mandatory, set to true to turn this mode on or false to turn it off.

recombination_mode_1 - Recombination between holes and electrons located at opposite sides of an interface. Boolean; mandatory, set to true to turn this mode on or false to turn it off.

generation_mode_0 - Generation within the bulk of materials. Boolean; mandatory, set to true to turn this mode on or false to turn it off.

generation_mode_0 - Generation at opposite sides of an interface. Boolean; mandatory, set to true to turn this mode on or false to turn it off.

Some features must explicitly be turned on since these require drastic changes in the equations which are being solved.

mid_gap_states - Enable calculation of mid-gap states at interfaces. more information about this will be added at a later time. Boolean; optional, default value false.

[numerics]

If a two-dimensional simulation is run, the numerical solution is found using a variant of the Gauss-Seidel method, called successive over-relaxation. The solution is considered to have converged when $\delta_a a_{n+1} < |a_{n+1} - a_n|$, where a_{n+1} is the $n+1$th iterative step, a the variable and δ_a the convergence criteria for the variable. In the case of one-dimensional simulations (set points_y = 1), the solution is instead found by the Thomas algorithm.

hole_convergence_criteria - The value of δ_a for the hole concentration. Decimal numbe; mandatory.

hole_relaxation_coefficient - The relaxation coefficient of the Gauss-Seidel method for the hole concentration solution. Decimal number; mandatory.

electron_convergence_criteria - The value of δ_a for the electron concentration. Decimal number; mandatory.

electron_relaxation_coefficient - The relaxation coefficient of the Gauss-Seidel method for the electron concentration solution. Decimal number; mandatory.

potential_convergence_criteria - The value of δ_a for the electric potential. Decimal number; mandatory.

potential_relaxation_coefficient - The relaxation coefficient of the Gauss-Seidel method for the electric potential solution. Decimal number; mandatory.

max_iteration_step - The maximum number of iterations before moving to the next data point even if the convergence criteria has not yet been fulfilled. Integer; mandatory.

initial_guess - The initial guess can either be from file, or simply a linearly potential drop. If this is set to "0", the program will try to read the initial guess from a file in the subfolder "initial_guess". The files (electron concentration, hole concentration and electric potential) must have the same names as those output by the program, e.g. electroncon_0, electroncon_1 and so on. If this is set to "1", the linear potential drop is used instead, requiring no other input. "0" or "1"; mandatory.

iterate_forward - If this is set to "true", the program uses the solution for the previous data point as initial guess for the next, ignoring the value of "initial_guess" after the first data point. Boolean; mandatory.

[electrode_n]

Make one section for each electrode in the simulation, with "n" being an integer starting from 0 ([electrode_0], [electrode_1]...). The only parameter than can be set for the electrodes is the work function, while parameters relating to the interface between semiconductors and the electrode are listed under a separate section.

lattice_number - The number corresponding to this electrode in the "lattice" file. Integer, mandatory.

work_function - The (positive) value for the work function of the electrode. Decimal number, mandatory.

[material_n]

Make one section for each material in the simulation, with "n" being an integer starting from 0 ([material_0], material_1]...). Some parameters relating to interfaces are found under a separate section.

lattice_number - The number corresponding to this material in the "lattice" file. Integer, mandatory.

hole_transport_energy - The energy at which the hole transport takes place in this material. Decimal number; mandatory.

electron_transport_energy - The energy at which the electron transport takes place in this material. Decimal number; mandatory.

mobility_hole - The mobility of holes in this material. Decimal number, mandatory.

mobility_electron - The mobility of electrons in this material. Decimal number, mandatory.

generation_rate - The effective rate of generated electrons and holes in the BULK of this material. The generation of free charge carriers can also be set to occur at donor/acceptor interface. Decimal number; mandatory.

relative_permittivity - The relative permittivity of this material. Decimal number; mandatory.

hole_transport_DOS - The effective density of states of the hole transport level in this material.

electron_transport_DOS - The effective density of states of the electron transport level in this material.

bulk_bimolecular_recombination_coef - The bimolecular recombination coefficient in the BULK of this material, optional, default value is that given by the Langevin theory.

bulk_reduced_recombination_coef - The reduction factor in the recombination rate in the BULK of this material. This should not be used in combination with a set value for the bulk bimolecular recombination coefficient, but if the default value is used, this makes it possible to adjust it without calculating the bimolecular recombination coefficient manually. Decimal number, optional, default value "1".

MG_minus_level - The energy level of mid-gap states, which are negatively charged when occupied. Decimal number, optional.

MG_plus_level - The energy level of mid-gap states, which are positively charged when occupied. Decimal number, optional.

MG_state_DOS - The effective density of states for the mid-gap state levels.

[material_interface_n]

Make one section for each pair of materials which are in contact with each other somewhere in the active layer, with "n" being an integer starting from 0 ([material_interface_0], material_interface_1]...). There is a separate section for electrode interfaces.

material_1 - The number corresponding to one of the two material in the "lattice" file. Integer, mandatory.

material_2 - The number corresponding to the other of the two material in the "lattice" file. Integer, mandatory.

hole_transport_energy - The energy at which holes are transported when moving across the interface. Decimal number; mandatory.

electron_transport_energy - The energy at which electrons are transported when moving across the interface. Decimal number; mandatory.

generation_rate - The effective generation rate of free charge carriers at this interface. Decimal number; mandatory.

relative_permittivity - The relative permittivity at the interface. Decimal number; mandatory.

hole_transport_DOS - The effective density of states of the hole transport level at the interface. Decimal number; mandatory.

electron_transport_DOS - The effective density of states of the electron transport level at the interface. Decimal number; mandatory.

interface_bimolecular_recombination_coef_1 - The bimolecular recombination coefficient across this interface between a hole located in material_1 and an electron in material_2, optional, default value is that given by the Langevin theory.

interface_bimolecular_recombination_coef_2 - The bimolecular recombination coefficient across this interface between a hole located in material_2 and an electron in material_1, optional, default value is that given by the Langevin theory.

interface_reduced_recombination_coef - The reduction factor in the recombination rate across this interface. This should not be used in combination with a set value for the bulk bimolecular recombination coefficient, but if the default value is used, this makes it possible to adjust it without calculating the bimolecular recombination coefficient manually. Decimal number, optional, default value "1".

[electrode_interface_n]

Make one section for each pair of material and electrode which are in contact with each other somewhere in the active layer, with "n" being an integer starting from 0 ([electrode_interface_0], electrode_interface_1]...).

material_number - The number corresponding to the material in the "lattice" file.

electrode_number - The number corresponding to the electrode in the "lattice" file.

boundary_condition - The options are simple ohmic contact (set this to 0), Schottky contact, where there may be a large dipole across this interface (set this to 1). "0" or "1"; mandatory.

surface_recombination - A selective layer can be replaced utilizing surface recombination velocity if this is set to true. Boolean; optional, default value false.

surface_recombination_velocity_electron - The surface recombination velocity for electrons at this interface. Decimal number, mandatory if surface_recombination is set to true for this interface.

surface_recombination_velocity_hole - The surface recombination velocity for hole at this interface. Decimal number, mandatory if surface_recombination is set to true for this interface.

[experiment]

A number of experiments have been implemented so far and more will be added if needed. Additionally, if one wishes to solve electrostatic problems, this is also an option.

iv - A simple IV-curve. Boolean; optional, default value false.

- **anode_potential_initial** - The voltage applied to the anode when the experiment is initiated.
- **cathode_potential_initial** - The voltage applied to the cathode when the experiment is initiated.
- **potential_step** - The amount by which the applied voltage is changed between data points.
- **data_points** - The number of data points in the IV-curve.

CELIV - A CELIV transient. Boolean; optional, default value false.

- **offset_voltage** - A constant voltage offset during the whole transient. Decimal number; optional, default value "0.0".
- **voltage_rise_speed** - The voltage rise speed of the linearly increasing voltage pulse. Decimal number, mandatory.
- **pulse_length** - The length of the voltage pulse. Decimal number, mandatory.
- **time_step** - The length of time between data points. This value must be sufficiently small, or numerical problems will ensue (significantly shorter than the time scale on which relevant processes occur). Decimal number, mandatory.
- **data_points** - The number of data points in the transient. Make sure that data_points $\times$ time_step $>$ pulse_length! Integer, mandatory.

transient_photocurrent - A transient photocurrent transient. Boolean; optional, default value false.

offset_voltage - A constant voltage offset during the whole transient. Decimal number; optional, default value "0.0".

pulse_length - The length of the voltage pulse. Decimal number, mandatory.

time_step - The length of time between data points. This value must be sufficiently small, or numerical problems will ensue (significantly shorter than the time scale on which relevant processes occur). Decimal number, mandatory.

data_points - The number of data points in the transient. Make sure that data_points × time_step > pulse_length! Integer, mandatory.

morphology_file

This file contains the morphology of the active layer, in the form of material numbers in a matrix-configuration. Each lattice point, for which the value of the charge carrier concentrations and electrical potential is calculated, is assigned the lattice number written down in the settings file. Points in the x-direction are separated by new lines and points in the y-direction by blank spaces. For example, a finger-structure, consisting of two different semiconductors, sandwiched between two electrodes with 10 lattice points in the x-direction and 6 in the y-direction would look like this:

3	3	3	3	3	3
1	1	1	1	1	1
1	1	1	2	2	2
1	1	1	2	2	2
1	1	1	2	2	2
1	1	1	2	2	2
1	1	1	2	2	2
1	1	1	2	2	2
2	2	2	2	2	2
4	4	4	4	4	4

Note that the simulation assumes periodic boundary conditions in the y-direction, therefore the electrodes need to be placed at x = 0 and x = points_x. It is of course possible to change the boundary conditions, but this is generally not straightforward. In the settings file, the lattice number for the two electrodes would be 3 and 4, and for the two semiconductors 1 and 2. The simulation will also require input for the interface between lattice number 1 and 2, as well as about the electrode interfaces between lattice number 3 and 1, as well as 2 and 4.

dopants_file

This file is constructed in a similar way as the morphology_file, but instead of using material number, the dopant concentration (in units of m^{-3}) should be written out for each lattice point. For example, using the morphology above, if the row of points closest to electrode 3 is p-doped with a concentration of $1 \times 10^{23}\mathrm{m}^{-3}$ negative ions, the file should contain the following:

0	0	0	0	0	0
−1E23	−1E23	−1E23	−1E23	−1E23	−1E23
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0

If the file name for the dopants file is not included in the settings file, the simulation assumes there are no dopants in any material. At some point, the option of providing a single, constant doping concentration for each material will be implemented, but for now, this is the only way of including doping.