# List of Parameters

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| --- | --- | --- | --- | --- | --- |
| **Variable Name** | **Parameter** | **(Default) Value** | **Units / Class** | **Comment** | **Input?** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Temp | Temperature | 300 | K |  | yes |
| AL\_thickness | Active Layer Thickness | 100\*1e-7 | cm |  | yes |

# Recombination Parameters

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Prec** | **Recombination Parameters** |  | **paramRec (class)** |  | yes |
| **Prec.const** | **Constants** |  | **struct** |  | **no** |
| Prec.const.kb | Boltzmann Constant | 8.6173e-05 | eV/K |  | no |
| Prec.const.me | Electron mass | 9.1000e-31 | kg |  | no |
| Prec.const.h | Planck’s constant | 6.6200e-34 | J / Hz |  | no |
| Prec.const.e | Elementary Charge | 1.6000e-19 | C | use literature value! | no |
| Prec.const.T | Temperature | 300 | K | It is not a constant, move it to params | yes |
| Prec.const.Edistribution | Energy distribution for luminescence spectra (still not sure what that means) | [1×501 double] | eV | The range is defined in paramsrec: const.Edistribution=0.5:0.005:3; %need to be linearly spaced | no |
| Prec.const.c | Speed of Light | 300000000 | m/s | use literature value! | no |
| Prec.const.eps0 | Vacuum permittivity | 6.9419e+08 = 4\*pi\*eps0 | eV / m | rename this, as it is not eps0 | no |
| Prec.const.solflux | Solar Spectrum  (Flux over Photon Energy) | [2002×2 double] | mA / (m^2 eV) | solflux(:,1) is the photon energy, solflux(:,2) is the solar flux | no |
| Prec.const.bb | Black Body Radiation | [501×2 double] | mA / (cm^2 eV) | = blackbody(T, Edistribution) | no |
| **Prec.params** | **Editable Recombination Parameters** |  | **struct** | **property of “Prec”** |  |
| Prec.params.thickness | Active Layer Thickness | 10e-7 | m |  | yes |
| Prec.params.sizeofsite | Electron Delocalization Radius | 5e-10 | m | size of exciton site calculated from density of exciton states in the active layer | yes |
| Prec.params.nie | Refractive Index | 1.5 | unitless |  | yes |
| Prec.params.RCTE | Ratio of CT states to Exciton States | 10 | unitless |  | yes |
| Prec.params.Vstar | Coupling between the LE and CT state (as defined in the JACS paper of flurin) | 1e-3 | eV |  | yes |
| Prec.params.offset | Energy offset between the LE and CT state | 0.1 | eV | Recalculated in the code | yes |
| **Prec.params.Ex /**  **Prec.params.CT** | **Exciton Parameters /**  **Charge Transfer State Parameters** |  | **struct** |  | **yes** |
| … .f | Oscillator strength | 5 / 0.05 | unitless |  | yes |
| … .L0 | Low frequency reorganisation energy | 0.1 / 0.18 | eV |  | yes |
| … .Li | High frequency reorganisation energy | 0.15 / 0.15 | eV |  | yes |
| … .DG0 | Free Energy of the transition from the ground state to the lowest exciton state. (Δ𝐺0𝐿𝐸) | 1.63 / 1.53 | ? |  | yes |
| … .Number\_Vibronic\_Mode\_initial | Vibronic mode for the initial state that are considered in the calculation | 5 | ? |  | yes |
| … .Number\_Vibronic\_Mode\_final | Vibronic mode for the final state that are considered in the calculation | 15 | ? |  | yes |
| … .hW | Vibronic mode energy of the effective mode considered in the calculations of the rates | 0.15 | eV |  | yes |
| … .sigma | Standard Deviation for the gaussian distribution of states | 0.02 / 0.04 | eV |  | yes |
| … .Dmus | Difference in static dipole moment | 3\*3.33e-30/1.6e-19 | e/meter | 3 in debye (\*3.33e-30 to get it in coulomb meter) then devided by q | yes |
| … .numbrestate | Number of excited states considered for the gaussian distribution | 5 |  | Number of states considered in the gaussian distribution | yes |
| … .S | Huang rhys factor | 1 | unitless | Calculated as Li/hW | yes |
| … .Gausswidth | Width of the Gaussian distribution | 0.1 / 0.2 |  | This is just to limit the integral used for the gaussian distribution. | yes |
| … .Statedistribution | Distribution of States | [1×5 double] | ? |  | yes |
| … .Znorm | Normalisation factor for the emission (see Jun’s PRL paper) | 3.57e-14 / 8.12e-12 | ? |  | yes |
| … .Znormabs | Normalisation factor for the absorption (see Jun’s PRL paper) | 0.0544 / 0.1088 | ? |  | yes |
| … .funlaguerre | laguerre function handles | [16×6 cell] |  | function in each cell is the same | yes |
| … .Dmu | Transition dipole moment ( calculated based on the oscillator strength and the energy of the transition) | 6.2158e-10 / 7.05e-11 | ? |  | yes |
| **… .results** | containing some resulting parameters | [1×1 struct] |  |  | no |
| … .results.FCWD0 | Franck condon weigthed density (sum) | [1 x 5 double] | eV-1 |  | no |
| … .results.FCWDEm | Franck condon weigthed density for emission (spectraly resolved) | [1 x 501 double] | eV-1 |  | no |
| … .results.FCWDabs | Franck condon weigthed density for absorption (spectraly resolved) | [1 x 501 double] | eV-1 |  | no |
| … .results.alphaLJ | Absorption coefficient | [1 x 501 double] | m-1 |  | no |
| … .results.knr | Non radiative Recombination rate constant of state | 1.1035e12 | s-1 |  | no |
| … .results.Hab | Electronic coupling | 0.3772 | eV |  | no |
| … .results.krTot | Radiative recombination rate constant | 1.7553e06 | s-1 |  | no |
| … .results.krE | Spectrally resolved radiative rate constant | [1 x 501 double] | eV-1s-1 |  | no |
| **Prec.results** | **Editable Recombination Parameters** |  | **struct** | **property of “Prec”** | no |
| Prec.results.Jscrad | Short Circuit Current (radiative?) | 24.25 | mA cm-2 | Max. Jsc if there were no losses due to recombination. | no |
| Prec.results.AbsLJ | Absorptivity of the Film | [1×501 double] | unitless | Similar to IQE of the device  (LJ = Levish Jortner Method, eq. 18 in the PRX paper) | no |
| Prec.results.alphaLJ | Absorption Coefficient | [1×501 double] | 1/m | see eq. 17 in the PRX paper | no |
| Prec.results.pe | Emission Probability | 0.2192 | unitless |  | no |
| Prec.results.J0rad | Radiative Dark Saturation Current | 4.9e-20 | mA cm-2 |  | no |
| Prec.results.Vocrad | Radiative Open Circuit Voltage Limit | 1.2317 | V |  | no |
| Prec.results.Qi | Internal luminescence quantum efficiency / Internal quantum yield of the EL emission (IQE\_LED) | 3.737e-5 | unitless | see eq. 5 PRX paper | no |
| Prec.results.Qe | External Quantum Efficiency of the Electroluminescence (Q\_LED) | 8.193e-6 | unitless | see eq. 4 PRX paper | no |
| Prec.results.Dvnr | Non-radiative voltage losses | 0.3028 | V | see eq. 6 PRX paper | no |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| krecCT | CT state recombination rate constant | Prec.params.CT.results.knr | s-1 |  | no |
| krecex | Exciton recombination rate constant | Prec.params.Ex.results.knr | s-1 |  | no |
| Voc | Open Circuit Voltage | results | V |  | no |

# Device Parameters

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| NC | Density of states  (?) Number of charge carriers (Electron/hole density)  This is defined here just as a way to access the N0V and N0C | 2e19 | 1/(cm3) |  |  |
| activelayer | Active Layer Index | 2 | Index | Indicates which layer is the active layer |  |
| mobility | charge carrier mobility | 3e-4 | cm2 / (V s) | for the active layer |  |
| Kfor | rate constant (CS to CT reformation) | 1e-10 | cm3s-1 | for the active layer |  |
| kdis | rate constant (CT dissociation) | 1.3e10 | cm3s-1 | for the active layer |  |
| kdisex | rate constant (Exciton dissociation) | 1e14 | cm3s-1 | for the active layer |  |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **DP** | **Device Parameters** |  | **deviceparams (class)** |  |  |
| **DP.physical\_const** | **Constants** |  |  | **Struct, property of «DP»** | no |
| DP.physical\_const.kB | Boltzmann Constant | 8.6173e-05 | eV/K |  | no |
| DP.physical\_const.T | Temperature | 300 | K |  | no |
| DP.physical\_const.epp0 | Vacuum Permittivity | 552434 | e^2 eV^-1 cm^-1 |  | no |
| DP.physical\_const.q | Charge normalised with the elementary charge | 1 | unitless |  | no |
| DP.physical\_const.e | Elementary Charge | 1.6192e-19 | C | use literature correctur value | no |
| **DP.solveropt** | **Options for the Differential Equation Solver** |  | **struct** |  | yes |
| DP.solveropt.AbsTol | Absolute Tolerance | 1e-6 | ? |  | yes |
| DP.solveropt.RelTol | Relative Tolerance | 1e-3 | ? |  | yes |
| DP.solveropt.m | System Geometry | 0 | 0, 1, or 2 | Define the geometry of the system (m=0 1D, m=1 cylindrical polar coordinates, m=2 spherical polar coordinates) | yes |
| DP.solveropt.options | contains even more options… | [1 x 1 struct] | struct |  | yes |
| **DP.pulse\_properties** | **Pulse Properties** |  | **struct** |  | yes |
| … .pulseon | Pulse on/off | 0 | Boolean (true/false) | Switch Pulse on for TPV | yes |
| … .pulselen | Transient Pulse length | 2e-10 | s |  | yes |
| … .tstart | Start time of Pulse | 1e-10 | s |  | yes |
| … .pulseint | Transient Pulse Intensity | 5 | sun equivalents | for BL and TM models, 100 mW/cm2 assumed | yes |
| **DP.light\_properties** | **Light Properties** |  | **struct** |  | yes |
| … .Int | Bias Light Intensity | 3 | sun equivalents |  | yes |
| … .OM | Optical Model | 0 | 0, 1, or 2 | 0 = uniform Generation,  1 = Beer-Lambert (Requires pre calculation using Igor code & gen profile in base workspace)  2 = Transfer Matrix (Standford) | yes |
| … .Genstrength | Generation Strength, number of photon absorbed( or exciton generated) under 1 sun. | 1.4981e22 | 1/cm^3 (for uniform generation) | Is recalculated based on the absorption of the device. | yes |
| **DP.Time\_properties** | **Time Properties** |  |  |  | yes |
| … .tmesh\_type | Time Mesh Type | 2 | Options: 1 or 2 | option 1: linear mesh  option 2: log space mesh (use this for pulsed laser light)  (correct?) | yes |
| … .tmax | Maximum Time for the simulation. | 5e-05 | s |  | yes |
| … .t0 | Time step size ( first time step suggested to the solver) | tmax/1000 | s |  | no |
| … tpoints | number of points in time mesh | 100 | integer number | in pnParamsHCT.m it is defined as 1000 ? is it overwritten by something else?  This is changed depending on the experiment check the different functions in device class. | yes |
| … .tmesh | time mesh | [1 x 100 double] | s ? |  | yes |
| **DP.Xgrid\_properties** | **Spatial Grid (along the X-coordinate)** | **[1 x 280 double]** | **??** |  | yes |
| **DP.layers\_num** | **Number of Layers** | **3** | **integer number** |  | yes |
| **DP.Experiment\_prop** | **Experiment Properties** |  |  |  | yes |
| … .Vapp | Applied Bias | 0 | V |  | yes |
| … .Vtransient | Transient Voltage (Step Size ?) | 0.01 | V |  | yes |
| … .wAC | ? | 1000 | ? |  | yes |
| … .fastrec | Fast recombination (yes / no) ? | 0 | Boolean (true/false) | Can be used to accelerate finding initial conditions | yes |
| … .BC | Boundary Conditions | 4 | ? | Must be set to one for first solution, BC=5 Impedance measurement | yes |
| … .figson | Toggle Figures on/off | 1 | Boolean (true/false) |  | yes |
| … .side | Illumination Side | 1 | 1 or 2 | 1 = EE (??)  2 = SE (??) | yes |
| … .calcJ | Calculate Current Options | 1 | 1 or 2 | slows down solving calcJ = 1, calculates DD currents at every position, calcJ = 2, calculates DD at boundary. | yes |
| … .mobset | Switch on/off electron hole mobility | 1 | boolean (true / false) | MUST BE SET TO ZERO FOR INITIAL SOLUTION | yes |
| … .symm | Using a symmetric model or not ( mainly used for ensuring that the device is held at open circuit voltage | 0 | ? |  | yes |
| … .equilibrium | System in Equilibrium (yes / no) ? | 0 | ? |  | yes |
| … .discretetrap | Consider discrete Traps (yes / no) ? | 0 | ? |  | yes |
| … .V\_fun\_type | Voltage function type | ‘constant’ | character vector | options: ‘constant’ / … ? | yes |
| … .V\_fun\_arg | Voltage function arguments | [0 1 5e-5] | V |  | yes |
| … .Vbi | Built in potential | 1.2049 | V |  | yes |
| **DP.layer\_colour** | **Layer Colour (for plotting?)** | **[6 x 3 double]** | **RGB ?** |  | **?** |
| **DP.results** | **Calculated Results** |  |  |  | no |
| DP.results.J0 | Dark saturation Current density | 6.03e-15 | mA cm-2 |  | no |
| DP.results.DVnr | Non-Radiative Voltage Loss | 0.3028 | V |  | no |
| DP.results.Voc | Open Circuit Voltage | 0.9289 | V |  | no |
| DP.results.Vocrad | Radiative Open Circuit Voltage Limit | 1.2317 | V |  | no |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **DP.Layers** |  |  | cell array of structs, one per layer | Imported from Excel!  Names in Excel Sheet below: | yes |
| DP.Layer{n}.epp | Dielectric Constant of the Layer | 1657302 | ? | Epp0 \* Epp (epp from excel) | yes |
| DP.Layer{n}.EA | Electron Affinity (Conduction Band Energy) | 0 | eV | ElectronAffinity | yes |
| DP.Layer{n}.IP | Ionisation Potential (Valence Band Energy) | -1.3049 | eV |  | yes |
| DP.Layer{n}.PhiCV | n doping (Energy shift) | 0 | eV |  | yes |
| DP.Layer{n}.PhiAV | p doping (Energy shift) | 0.05 | eV |  | yes |
| DP.Layer{n}.N0C | Effective Density of States at the Conduction Band | 2e19 | 1/(cm^3) | N0C | yes |
| DP.Layer{n}.N0V | Effective Density of States at the Valence Band | 2e19 | 1/(cm^3) | N0V | yes |
| DP.Layer{n}.muee | Electron mobility | 1e-03 | cm2 / (V s) | Imported Value | yes |
| DP.Layer{n}.mupp | Hole mobility | 10 | cm2 / (V s) | Imported Value | yes |
| DP.Layer{n}.krad | radiative recombination rate? | 1e-13 | cm3s-1 | NEEDS to be removed from the code (according to your comment) | yes |
| DP.Layer{n}.taun | SRH time constant for electrons | 1 | s |  | yes |
| DP.Layer{n}.taup | SRH time constant for holes | 1 | s |  | yes |
| DP.Layer{n}.Ete | Energy of the Trap States (Electrons) | -0.5 | eV ? | ((EA-IP)/2+IP)-0.2 Deep trap energy is currently a guess! | yes |
| DP.Layer{n}.Eth | Energy of the Trap States (Holes) | -0.5 | eV ? |  | yes |
| DP.Layer{n}.NTA | Density of Trap States (Acceptor) | 1e10 | 1/cm^3 |  | yes |
| DP.Layer{n}.NTD | Density of Trap States (Donor) | 1e10 | 1/cm^3 |  | yes |
| DP.Layer{n}.tp | Layer Thickness | 1e-5 | cm |  | yes |
| DP.Layer{n}.pp | Number of Points int the Layer | 20 | Integer |  | yes |
| DP.Layer{n}.tinterL | Interfacial Region Thickness (Left) | 0 | m ? cm ? |  | yes |
| DP.Layer{n}.epointsL | number of points in the left interlayer | 0 | integer | No. of points for electrode [for log mesh] | yes |
| DP.Layer{n}.XiL | Interfacial region thickness Heterojunction (left) | 0 | m? cm? |  | yes |
| DP.Layer{n}.XipL | number of points in the left heterojunction interlayer | 0 | integer | No. of points for electrode [for log mesh] | yes |
| DP.Layer{n}.tinterR | Interfacial Region Thickness (Right) | 2.5e-6 | m ? cm ? |  | yes |
| DP.Layer{n}.epointsR | number of points in the right interlayer | 25 | integer | No. of points for electrode [for log mesh] | yes |
| DP.Layer{n}.XiR | Interfacial region thickness Heterojunction (right) | 1e-7 | m ? cm ? |  | yes |
| DP.Layer{n}.XipR | number of points in the right heterojunction interlayer | 10 | integer | No. of points for electrode [for log mesh] | yes |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
| DP.Layer{n}.int | Intensity | 1 | Sun equivalents | Used to define if the layer absorbs light | yes |
| DP.Layer{n}.kdisexc | rate constant (Exciton dissociation) | 1e12 | s-1 |  | yes |
| DP.Layer{n}.kdis | rate constant (CT dissociation) | 3 | s-1 |  | yes |
| DP.Layer{n}.kfor | rate constant (CS to CT reformation) | 1e-10 | cm3s-1 | why is this one a different unit compared to the other rate constants? | yes |
| DP.Layer{n}.krec | rate constant (CT recombination) | 3e12 | s-1 |  | yes |
| DP.Layer{n}.kforEx | rate constant (CT to Exciton) | 2.0897e11 | s-1 |  | yes |
| DP.Layer{n}.krecexc | rate constant (Exciton recombination) | 6.3603e09 | s-1 |  | yes |
| DP.Layer{n}.PhiC | ? | 0 | ? |  | yes |
| DP.Layer{n}.PhiA | ? | -1.2549 | ? | calculated from IP-PhiAV | yes |
| DP.Layer{n}.Eg | Band Gap (?) | 1.3049 | eV ? |  | yes |
| DP.Layer{n}.mue | Electron Mobility | 1e-3 | cm^2 / (V s) | value that is used by code | yes |
| DP.Layer{n}.mup | Hole Mobility | 10 | cm^2 / (V s) | value that is used by code | yes |
| DP.Layer{n}.ni | Intrinsic Charge Carrier Density | 2.8911e18 | cm^-3 ? |  | yes |
| DP.Layer{n}.n0 | Density of Electrons at Equilibrium | 0.0166 | cm^-3 ? |  | yes |
| DP.Layer{n}.p0 | Density of Holes at Equilibrium | 2.8911e18 | cm^-3 ? |  | yes |
| DP.Layer{n}.c0 | Density of Cations at Equilibrium | 0.0017 | cm^-3 | CAN BE REMOVED | yes |
| DP.Layer{n}.Phi | Fermi Level | -1.2549 | eV ? |  | yes |
| DP.Layer{n}.ND | Dopant Density (Donor) | 0 | cm^-3 ? m^-3 ? |  | yes |
| DP.Layer{n}.NA | Dopant Density (Acceptor) | 2.8911e18 | cm^-3 ? m^-3 ? |  | yes |
| DP.Layer{n}.Ei | Intrinsic Fermi Level | -0.6525 | eV |  | yes |
| DP.Layer{n}.nt | Density of CB electrons when Fermi level at trap state energy | 7.9689e10 | cm^-3 ? m^-3 ? | CB = conduction band | yes |
| DP.Layer{n}.pt | Density of VB holes when Fermi level at trap state energy | 6.0158e05 | cm^-3 ? m^-3 ? | VB = valence band | yes |
| DP.Layer{n}.en | Trap property (electron) | 7.9689 | ? |  | yes |
| DP.Layer{n}.Cn | Trap property (electron) | 1e-10 | ? |  | yes |
| DP.Layer{n}.ep | Trap property (hole) | 6.0158e-5 | ? |  | yes |
| DP.Layer{n}.Cp | Trap property (hole) | 1e-10 | ? |  | yes |
| DP.Layer{n}.CT0 | Density of CT states (at equilibrium) | 1.598e6 | cm^-3 ? m^-3 ? | CT = Charge Transfer | yes |
| DP.Layer{n}.Ex0 | Density of Ex states (at equilibrium) | 3.3392e5 | cm^-3 ? m^-3 ? | EX = Exciton | yes |
| DP.Layer{n}.DEAR | Derivative of the Electron Affinity (right side of the layer) | 0 | ? | For the Heterojunction | yes |
| DP.Layer{n}.DIPR | Derivative of the Ionisation Potential (right side of the layer) | 0 | ? | For the Heterojunction | yes |
| DP.Layer{n}.DN0CR | Derivative of the Effective density of states at the Conduction band (right) | 0 | ? | For the Heterojunction | yes |
| DP.Layer{n}.DN0VR | Derivative of the Effective density of states at the Valence band (right) | 0 | ? | For the Heterojunction | yes |
| DP.Layer{n}.XL | Left Position (Start of the Layer) | 0 | cm |  | yes |
| DP.Layer{n}.XR | Right Position (End of the Layer) | 5e-6 | cm |  | yes |

**Layer Parameters (Excel)**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Epp |  |  |  |  | yes |
| Electron Affinity |  |  |  |  | yes |
| Valenceband |  |  |  |  | yes |
| ndoping |  |  |  |  |  |
| pDoping |  |  |  |  |  |
| N0C |  |  |  |  |  |
| N0V |  |  |  |  |  |
| mue |  |  |  |  |  |
| Mup |  |  |  |  |  |
| Krad |  |  |  |  |  |
| Taun |  |  |  |  |  |
| Taup |  |  |  |  |  |
| Ete |  |  |  |  |  |
| Eth |  |  |  |  |  |
| DensityOfAcceptorTrapStates |  |  |  |  |  |
| DensityOfDonorTrapStates |  |  |  |  |  |
| tp |  |  |  |  |  |
| pp |  |  |  |  |  |
| tinterL |  |  |  |  |  |
| epointsL |  |  |  |  |  |
| XiL |  |  |  |  |  |
| XipL |  |  |  |  |  |
| tinterD |  |  |  |  |  |
| epointsD |  |  |  |  |  |
| XiD |  |  |  |  |  |
| XipD |  |  |  |  |  |
| wr |  |  |  |  |  |
| wl |  |  |  |  |  |
| int |  |  |  |  |  |
| kdisexc |  |  |  |  |  |
| kdis |  |  |  |  |  |
| kfor |  |  |  |  |  |
| krec |  |  |  |  |  |
| kforex |  |  |  |  |  |
| krecex |  |  |  |  |  |



Interfacial layer for the cases where we have a heterojunction ( change in the energy levels or the density of states)

Number of points is XipL and thickness is XiL

layer with more points than the bulk to better assess the changes between the layers due to changes in the properties.

tinterL :thickness

EpointsL: number of points

Rest of the layer. Number of points is pp