# List of Parameters

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

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

# Recombination Parameters

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Prec** | **Recombination Parameters** | **NaN** | **NaN** | **Object of «paramsRec» Class** | yes |
| **Prec.const** | **Constants** | **NaN** | **NaN** | **Struct, property of «Prec»** | **no** |
| Prec.const.V | ?? | 30 | ?? |  | 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 |  | no |
| Prec.const.T | Temperature | 300 | K | why do we define this twice? | yes |
| Prec.const.Edistribution | ??? | [1×501 double] | ? |  | no |
| Prec.const.c | Speed of Light | 300000000 | ? |  | no |
| Prec.const.eps0 | Vacuum permittivity | 6.9419e+08 ??? | ??? | i could not find this value for the vacuum permittivity anywhere in the literature | 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 | ??? | [501×2 double] | ? |  | ? |
| Prec.const.chemicalpot | Chemical Potential of ??? | 0.9000 | ? |  | ? |
| **Prec.params** | **Editable Recombination Parameters** |  | **struct** | **property of “Prec”** |  |
| Prec.params.thickness | Active Layer Thickness | AL\_thickness\*1e-2  = 10e-7 | m ? | why don’t we just define it only here? | yes |
| Prec.params.sizeofsite | electron delocalization radius (?) | 5e-10 | m ? cm ? |  | yes |
| Prec.params.nie | Refractive Index (ie ?) | 1.5 | struct |  | yes |
| Prec.params.RCTE | ??? | 10 | struct |  | yes |
| Prec.params.Vstar | ??? | 1e-3 | struct |  | yes |
| Prec.params.offset | ??? | 0.1 | struct |  | yes |
| **Prec.params.Ex /**  **Prec.params.CT** | **Exciton Parameters /**  **Charge Transfer State Parameters** |  | struct |  | yes |
| … .f |  | 5 / 0.05 |  |  | yes |
| … .L0 |  | 0.1 / 0.18 |  |  | yes |
| … .Li |  | 0.15 / 0.15 |  |  | yes |
| … .DG0 | Free Energy of the transition from the ground state to the lowest exciton state. (Δ𝐺0𝐿𝐸) | 1.63 / 1.53 |  |  | yes |
| … .ModeCT |  | 5 |  |  | yes |
| … .ModeGS |  | 15 |  |  | yes |
| … .hW |  | 0.15 |  |  | yes |
| … .sigma |  | 0.02 / 0.04 |  |  | yes |
| … .Dmus |  | 6.24e-11 / 2.08e-10 |  |  | yes |
| … .numbrestate |  | 5 |  |  | yes |
| … .S |  | 1 |  |  | yes |
| … .Gausswidth |  | 0.1 / 0.2 |  |  | yes |
| … .Statedistribution |  | [1×5 double] |  |  | yes |
| … .Znorm |  | 3.57e-14 / 8.12e-12 |  |  | yes |
| … .Znormabs |  | 0.0544 / 0.1088 |  |  | yes |
| … .funlaguerre | laguerre function handles | [16×6 cell] |  | function in each cell is the same | yes |
| … .Dmu |  | 6.2158e-10 / 7.05e-11 |  |  | yes |
| **… .results** | containing some resulting parameters | [1×1 struct] |  |  | no |
| … .results.FCWD0 |  |  |  |  | no |
| … .results.FCWDEm |  |  |  |  | no |
| … .results.FCWDabs |  |  |  |  | no |
| … .results.alphaLJ |  |  |  |  | no |
| … .results.knr | Recombination rate constant |  |  |  | no |
| … .results.Hab |  |  |  |  | no |
| … .results.krTot |  |  |  |  | no |
| … .results.krE |  |  |  |  | no |
| **Prec.results** | **Editable Recombination Parameters** |  | **struct** | **property of “Prec”** | no |
| Prec.results.Jscrad | Short Circuit Current (radiative?) | 24.25 | ?? |  | no |
| Prec.results.AbsLJ | ?? | [1×501 double] |  |  | no |
| Prec.results.alphaLJ | ?? | [1×501 double] |  |  | no |
| Prec.results.pe | Emission Probability | 0.2192 |  |  | no |
| Prec.results.J0rad | Radiative Dark Saturation Current | 4.9e-20 |  |  | no |
| Prec.results.Vocrad | Radiative Open Circuit Voltage Limit | 1.2317 |  |  | no |
| Prec.results.Qi | ?? | 3.737e-5 |  |  | no |
| Prec.results.Qe | ?? | 8.193e-6 |  |  | no |
| Prec.results.Dvnr | ?? | 0.3028 | V |  | 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 | (?) Number of charge carriers (Electron/hole density) | 2e19 | cm-3 |  |  |
| activelayer | Active Layer Index | 2 | Index |  |  |
| Kfor | ?? | 1e-11 | ?? |  |  |
| mobility | charge carrier mobility | 3e-4 | cm^2 / (V s) |  |  |
| kdis | CT(??) dissociation rate constant | 1.3e10 | ? |  |  |
| kdisex | Exciton dissociation rate constant | 1e14 | ? |  |  |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **DP** | **Device Parameters** |  |  | **object of the class pnParamsHCT** |  |
| **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 | doesn’t agree with value above | no |
| DP.physical\_const.q | Charge normalised with the elementary charge | 1 | unitless |  | no |
| DP.physical\_const.e | Elementary Charge | 1.6192e-19 | C |  | 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** |  |  |  | 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 | mW/cm2 | for BL and TM models, 100 mW/cm2 assumed | yes |
| **DP.light\_properties** | **Light Properties** |  |  |  | yes |
| … .Int | Bias Light Intensity | 3 | Suns ?? |  | 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 (??) | 1.4981e22  defined value 2.5e21 is overwritten! | cm-3 | for uniform generation in cm-3 | yes |
| **DP.Time\_properties** | **Time Properties** |  |  |  | yes |
| … .tmesh\_type | Time Mesh Type | 2 | ?? | selection out of ?? | yes |
| … .tmax | Maximum Time ? | 5e-05 | ?? |  | yes |
| … .t0 | Time step size? | tmax/1000 | ?? |  | 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? | yes |
| … .tmesh | time mesh | [1 x 100 double] | ?? |  | 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 | ? | 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] | ? |  | yes |
| … .Vbi | ? | 1.2049 | ? |  | yes |
| **DP.layer\_colour** | **Layer Colour (for plotting?)** | **[6 x 3 double]** | **RGB ?** |  | **?** |
| **DP.results** | **Calculated Results** |  |  |  | no |
| DP.results.J0 | Dark Current | 6.03e-15 | mA … ? |  | 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 |  | 1657302 | ? | Epp | yes |
| DP.Layer{n}.EA | Electron Affinity | 0 | ? | ElectronAffinity | yes |
| DP.Layer{n}.IP | Ionisation Potential | -1.3049 | ? | ? | yes |
| DP.Layer{n}.PhiCV |  | 0 | ? |  | yes |
| DP.Layer{n}.PhiAV |  | 0.05 | ? |  | yes |
| DP.Layer{n}.N0C | ? | 2e19 | ? | N0C | yes |
| DP.Layer{n}.N0V | ? | 2e19 | ? | N0V | yes |
| DP.Layer{n}.muee | Electron mobility | 1e-03 | cm^2 / (V s) | mue ? why twice? see below | yes |
| DP.Layer{n}.mupp | Hole mobility | 10 | cm^2 / (V s) | Mup ? why twice? see below | yes |
| DP.Layer{n}.krad | radiative recombination rate? | 1e-13 | ? |  | yes |
| DP.Layer{n}.taun | n-type tau ? (what is tau?) | 1 | ? |  | yes |
| DP.Layer{n}.taup | p-type tau ? (what is tau?) | 1 | ? |  | yes |
| DP.Layer{n}.Ete |  | -0.5 | ? |  | yes |
| DP.Layer{n}.Eth |  | -0.5 | ? |  | yes |
| DP.Layer{n}.NTA |  | 1e10 | ? |  | yes |
| DP.Layer{n}.NTD |  | 1e10 | ? |  | yes |
| DP.Layer{n}.tp | Layer Thickness ? | 1e-5 | cm? | doesn’t agree with Prec.params.tickness !! Different units maybe? | yes |
| DP.Layer{n}.pp |  | 20 | ? |  | yes |
| DP.Layer{n}.tinterL | thickness left interlayer | 0 | ? |  | yes |
| DP.Layer{n}.epointsL | number of points in the left interlayer | 0 | ? |  | yes |
| DP.Layer{n}.XiL | ?? left interlayer | 0 | ? |  | yes |
| DP.Layer{n}.XipL | ?? left interlayer | 0 | ? |  | yes |
| DP.Layer{n}.tinterR | thickness right interlayer | 2.5e-6 | ? |  | yes |
| DP.Layer{n}.epointsR | number of points in the right interlayer | 25 | ? |  | yes |
| DP.Layer{n}.XiR | ?? right interlayer | 1e-7 | ? |  | yes |
| DP.Layer{n}.XipR | ?? right interlayer | 10 | ? |  | yes |
| DP.Layer{n}.wr | ? | 2e-6 | ? |  | yes |
| DP.Layer{n}.wl | ? | 0 | ? |  | yes |
| DP.Layer{n}.int | intensity? | 1 | ? |  | 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 |  | 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 | ? |  | yes |
| DP.Layer{n}.Eg | Band Gap (?) | 1.3049 | eV ? |  | yes |
| DP.Layer{n}.mue | Electron Mobility | 1e-3 | cm^2 / (V s) | mue ? why twice? | yes |
| DP.Layer{n}.mup | Hole Mobility | 10 | cm^2 / (V s) | Mup ? why twice? | yes |
| DP.Layer{n}.ni | ? | 2.8911e18 | ? |  | yes |
| DP.Layer{n}.n0 | ? | 0.0166 | ? |  | yes |
| DP.Layer{n}.p0 | ? | 2.8911e18 | ? |  | yes |
| DP.Layer{n}.c0 | ? | 0.0017 | ? |  | yes |
| DP.Layer{n}.Phi | ? | -1.2549 | ? |  | yes |
| DP.Layer{n}.ND | ? | 0 | ? |  | yes |
| DP.Layer{n}.NA | ? | 2.8911e18 | ? |  | yes |
| DP.Layer{n}.Ei | ? | -0.6525 | ? |  | yes |
| DP.Layer{n}.nt | ? | 7.9689e10 | ? |  | yes |
| DP.Layer{n}.pt | ? | 6.0158e05 | ? |  | yes |
| DP.Layer{n}.en | ? | 7.9689 | ? |  | yes |
| DP.Layer{n}.Cn | ? | 1e-10 | ? |  | yes |
| DP.Layer{n}.ep | ? | 6.0158e-5 | ? |  | yes |
| DP.Layer{n}.Cp | ? | 1e-10 | ? |  | yes |
| DP.Layer{n}.CT0 | ? | 1.598e6 | ? |  | yes |
| DP.Layer{n}.Ex0 | ? | 3.3392e5 | ? |  | yes |
| DP.Layer{n}.DEAR | ? | 0 | ? |  | yes |
| DP.Layer{n}.DIPR | ? | 0 | ? |  | yes |
| DP.Layer{n}.DN0CR | ? | 0 | ? |  | yes |
| DP.Layer{n}.DN0VR | ? | 0 | ? |  | yes |
| DP.Layer{n}.XL | ? | 0 | ? |  | yes |
| DP.Layer{n}.XR | ? | 5e-6 | ? |  | 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 |  |  |  |  |  |