In[229]:=
```
Needs["NumericalCalculus`"]
```

Physical Constants and Parameters

Length units are cm, mass is gram, time is second, energy is eV, current is mA

Constants

In[230]:=
```
c = 3 × 10^10; (*speed of light*)
h = 4.14 × 10^-15; (*Planck constant, eVs*)
kB = 8.62 × 10^-5; (*Boltzmann constant, eV/K*)
T = 300;
kBT = kB * T;
q = 1.602 × 10^-16; (*fundamental charge, mC*)
```

GaAs properties

Take convention that valence band edge energy is E=0

In[236]:=
```
cbb = 1.3 × 10^-10; (*GaAs radiative recombination coefficient*)
ni = 2 × 10^6; (*GaAs intrinsic carrier concentration*)
p_emit = 10.0 × 10^19; (*Emitter doping density*)
eu = 1.0 × 10^-3 * (12 + 6 * p_emit / 10^19) (*Linear fit to Urbach Energy vs doping*)
nv = 9.0 × 10^18; (*valence band density of states*)
nc = 4.7 × 10^17; (*conduction band density of states*)
n = 3.5 (*Band edge index of refraction*);
eg = 1.42; (*unperturbed bandgap*)
eg_emit = eg - 1.6 × 10^-8 p_emit^1/3 (*Bandgap narrowing of the emitter*)
α_bandgap = 1000.0; (*Absorption at the bandgap below which
 is band tails. Used for scaling the absorption calculation*)
Dn = 35 + 28 * Log[p_emit / 10^19]; (*Electron diffusion coefficient,
important if using surface recombination*)
srv = 5 × 10^7; (*Electron surface recombination velocity*)
```

Out[239]=
```
0.072
```

Out[244]=
```
1.34573
```

Fermi-Dirac and Bose-Einstein Distributions

In[248]:=

$$fd[e\_?NumericQ, \mu\_?NumericQ] := \frac{1}{Exp[(e-\mu)/kBT]+1}$$

$$be[e\_?NumericQ, \mu\_?NumericQ] := \frac{1}{Exp[(e-\mu)/kBT]-1}$$

Find the Hole Fermi level and equilibrium electron concentration

In[250]:=

$$p[efp\_?NumericQ] := nv\,\frac{2}{Sqrt[Pi]}\,NIntegrate[Sqrt[-e/kBT]\,(1-fd[e, efp])/kBT, \{e, -Infinity, 0\}]$$

In[251]:=

```
efp = FindRoot[p[x] == p_emit, {x, 0}, PrecisionGoal → 4][[1, 2]]
np0 = nc Exp[-(eg_emit - efp)/kBT]
```

Out[251]=

$$-0.151961$$

Out[252]=

$$3.30902\times10^{-8}$$

Device geometry

In[253]:=

```
We = 200.0 × 10^-7; (*Emitter Width*)
Wd = 200.0 × 10^-7; (*Depletion Width*)
Lp = 10.0 × 10^-4; (*Base Width*)
```

Calculate the electron QFL and QFL splitting

In[256]:=

```
Ln = 1.7 × 10^-4 (p_emit / 10^19)^-0.4
  (*electron diffusion length, https://doi.org/10.1063/1.109997*)
```

Out[256]=

$$0.0000676782$$

In[257]:=

```
n_edge[v__?NumericQ] := nc * Exp[-(eg_emit - (efp + v)) / kBT];
(*electron density at edge of depletion*)
n_emit[x__?NumericQ, v__?NumericQ] := (2 e^(We/Ln) (Dn np0 Cosh[We/Ln] +
        Ln np0 srv Sinh[We/Ln] - (np0 - n_edge[v]) (Dn Cosh[x/Ln] + Ln srv Sinh[x/Ln])))/
    (Dn - Ln srv + e^(2 We/Ln) (Dn + Ln srv));(*Analytic solution of diffusion equation*)
efn[x__?NumericQ, v__?NumericQ] := kBT * Log[n_emit[x, v]/nc] + eg_emit;
j_surf[v__?NumericQ] := q * Dn * (-np0 + n_edge[v]) srv / (Dn Cosh[We/Ln] + Ln srv Sinh[We/Ln]);
Δμ[x__?NumericQ, v__?NumericQ] := efn[x, v] - efp;
```

Simulation settings

In[262]:=

```
dv = 0.001;(*voltage resolution for i-v calculations*)
vmax = 1.2;
vmin = -0.1;
jl = -30; (*Photocurrent. Adopt convention
 that forward bias is positive diode current*)
psun = 100;(*AM1.5G*)
e0 = 0;(*grid settings for pre-computing absorption coefficient*)
emax = eg_emit + 0.3;
de = 0.005;
Δμ0 = 0;
Δμmax = emax;
dΔμ = 0.005;
```

Helper Functions

In[273]:=

```
calc_pmax[j_] := NMaximize[{-x * j[x], x ≥ vmin, x ≤ vmax}, x, PrecisionGoal → 4]
calc_eff[j_] := calc_pmax[j] / psun
calc_jsc[j_] := j[0]
calc_voc[j_] := FindRoot[j[x], {x, 0.5 * (vmin + vmax)}]
calc_ff[j_] := calc_pmax[j] / (calc_jsc[j] * calc_voc[j])
calc_ideality[j_, v_] := kBT^-1 ((Log[j[v + dv]] - Log[j[v]]) / dv)^-1
calc_pv[j_] := Module[{cell_pmax, cell_eff, cell_jsc, cell_voc, cell_ff,
    cell_vmpp, cell_jmpp, cell_ideal, pmax, vmpp, jmpp, eff, jsc, voc, ff, ideal},
  cell_pmax = calc_pmax[j];
  cell_vmpp = cell_pmax[[2, 1, 2]];
  cell_pmax = cell_pmax[[1]];
  cell_jmpp = j[cell_vmpp];
  cell_eff = cell_pmax / psun;
  cell_jsc = -calc_jsc[j];
  cell_voc = calc_voc[j][[1, 2]];
  cell_ff = cell_pmax / (cell_jsc * cell_voc);
  Return[<|
    "pmax" → cell_pmax,
    "vmpp" → cell_vmpp,
    "jmpp" → cell_jmpp,
    "eff" → cell_eff,
    "jsc" → cell_jsc,
    "voc" → cell_voc,
    "ff" → cell_ff|>]]
```

Depletion and Base Current

In[280]:=

$$\text{jdb\_dark}[v\_\_?\text{NumericQ}] := \text{Piecewise}\left[\{\{0, v == 0\}\}, q\, cbb\, ni^2 \left(Wd\,(\text{Exp}[v/kBT] - 1) - Lp + Lp\,\frac{kBT}{v}\,(\text{Exp}[v/kBT] - 1)\right)\right]$$

In[281]:=

```
jdb_light[v__?NumericQ] := jl + jdb_dark[v]
```

Reproduce a good GaAs cell photovoltaic parameters

In[282]:=
```
good_pv = calc_pv[jdb_light]
calc_ideality[jdb_dark, good_pv["vmpp"]]
```

Out[282]=
```
⟨| pmax → 30.1315, vmpp → 1.02996, jmpp → -29.2551,
 eff → 0.301315, jsc → 30, voc → 1.1268, ff → 0.891363 |⟩
```

Out[283]=
```
1.01416
```

Emitter Current

Integrand for calculating the Urbach absorption. Have already implicitly used Dirac function to integrate ec.

In[284]:=
```
α_integrand[ev_?NumericQ, Δμ_?NumericQ, e_?NumericQ] :=
 Re[Sqrt[-ev]] Exp[(ev + e) / eu] (fd[ev, efp] - fd[ev + e, efp + Δμ])
```

In[285]:=
```
α_factor = α_bandgap / NIntegrate[α_integrand[ev, 0, eg_emit], {ev, -Infinity, 0}];
```

In[286]:=
```
α[e__?NumericQ, Δμ__?NumericQ] := Piecewise[{
    {α_factor * NIntegrate[α_integrand[ev, Δμ, e], {ev, -Infinity, 0}, PrecisionGoal → 4,
       AccuracyGoal → 4, MaxRecursion → 20, Method → "LocalAdaptive"],
     e < eg_emit},
    {α_bandgap,
     e ≥ eg_emit}
  }]
```

Pre compute absorption spectra and turn into interpolating function

In[287]:=
```
(*α_table=
 Flatten[Parallelize[Table[{{e,Δμ},α[e,Δμ]},{Δμ,Δμ0,Δμmax,dΔμ},{e,e0,emax,de}]],1];
α_interpf=Interpolation[α_table,InterpolationOrder→2];*)
α_interp[e_?NumericQ, Δμ_?NumericQ] := α_interpf[e, Δμ];
```

Black body photon flux

In[288]:=
$$\text{jbb}[e\_?\text{NumericQ}, \Delta\mu\_?\text{NumericQ}] := \frac{8\,\text{Pi}\,n^2\,c}{(h\,c)^3}\,e^2 * \text{be}[e, \Delta\mu];$$

In[289]:=
```
current_integrand[e_?NumericQ, Δμ_?NumericQ] := α_interp[e, Δμ] * jbb[e, Δμ]
```

In[290]:=
```
emitter_current_density[Δμ_?NumericQ] :=
 q * NIntegrate[current_integrand[e, Δμ], {e, 0, emax},
   PrecisionGoal → 3, MaxRecursion → 20, Method → "LocalAdaptive"]
```

In[291]:=
```
emitter_current[v_?NumericQ] := NIntegrate[emitter_current_density[Δμ[x, v]],
  {x, 0, We}, PrecisionGoal → 3, MaxRecursion → 20, Method → "LocalAdaptive"]
```

In[292]:=
```
cellj_dark[v_?NumericQ] := jdb_dark[v] + emitter_current[v] + j_surf[v]
cellj_light[v_?NumericQ] := cellj_dark[v] + jl
(*cellj_light_table=Parallelize[Table[{v,cellj_light[v]},{v,vmin,vmax,dv}]];
cellj_light_interpf=Interpolation[cellj_light_table,InterpolationOrder→1];*)
cellj_light_interp[v_?NumericQ] := Piecewise[{
    {cellj_light_interpf[vmin], v < vmin},
    {cellj_light_interpf[vmax], v > vmax}
   },
   cellj_light_interpf[v]
  ];
```

In[295]:=
```
initialize[doping_] := Module[{},
  p_emit = doping;
  Dn = 35 + 28 * Log[p_emit / 10^19];
  eu = 1.0 × 10^-3 * (12 + 6 * p_emit / 10^19);
  (*Linear fit to Urbach Energy vs doping*)
  eg_emit = eg - 1.6 × 10^-8 p_emit^1/3; (*Bandgap narrowing of the emitter*)
  efp = FindRoot[p[x] == p_emit, {x, 0}][[1, 2]];
  np0 = nc Exp[-(eg_emit - efp) / kBT];
  Ln = 1.7 × 10^-4 (p_emit / 10^19)^-0.4;
  α_factor = α_bandgap / NIntegrate[α_integrand[ev, 0, eg_emit], {ev, -Infinity, 0}];
  α_table = Flatten[
    Parallelize[Table[{{e, Δμ}, α[e, Δμ]}, {Δμ, Δμ0, Δμmax, dΔμ}, {e, e0, emax, de}]], 1];
  α_interpf = Interpolation[α_table, InterpolationOrder → 2];
  cellj_light_table = Parallelize[Table[{v, cellj_light[v]}, {v, vmin, vmax, dv}]];
  cellj_light_interpf = Interpolation[cellj_light_table, InterpolationOrder → 1];
 ]
```

In[296]:=
```
For[val = 1.0 × 10^19, val ≤ 10.0 × 10^19, val = val + 1.0 × 10^19,
 Print[val];
 initialize[val];
 cell_pv = calc_pv[cellj_light_interp];
 Print[cell_pv];
 Print[calc_ideality[cellj_dark, cell_pv["vmpp"]]];
]
```

$1. \times 10^{19}$

FindRoot: The line search decreased the step size to within tolerance specified by AccuracyGoal and PrecisionGoal but was unable to find a sufficient decrease in the merit function. You may need more than MachinePrecision digits of working precision to meet these tolerances.

```
⟨| pmax → 26.5519, vmpp → 0.91, jmpp → -29.1779,
 eff → 0.265519, jsc → 30., voc → 1.00303, ff → 0.882386 |⟩
```

```
1.00016
```

```
2. × 10^19
```

```
⟨| pmax → 26.7301, vmpp → 0.916, jmpp → -29.1814,
 eff → 0.267301, jsc → 30., voc → 1.00927, ff → 0.882825 |⟩
```

```
1.00108
```

```
3. × 10^19
```

```
⟨| pmax → 26.5849, vmpp → 0.913, jmpp → -29.1182,
 eff → 0.265849, jsc → 30., voc → 1.00864, ff → 0.878572 |⟩
```

```
1.05013
```

```
4. × 10^19
```

••• FindRoot: The line search decreased the step size to within tolerance specified by AccuracyGoal and PrecisionGoal but was unable to find a sufficient decrease in the merit function. You may need more than MachinePrecision digits of working precision to meet these tolerances.

```
⟨| pmax → 25.2845, vmpp → 0.874154, jmpp → -28.9245,
 eff → 0.252845, jsc → 30., voc → 0.982503, ff → 0.857824 |⟩
```

```
1.27109
```

```
5. × 10^19
```

```
⟨| pmax → 23.3381, vmpp → 0.814, jmpp → -28.6709,
 eff → 0.233381, jsc → 30., voc → 0.933013, ff → 0.833789 |⟩
```

```
1.46135
```

```
6. × 10^19
```

```
⟨| pmax → 21.3548, vmpp → 0.752, jmpp → -28.3973,
 eff → 0.213548, jsc → 30., voc → 0.877387, ff → 0.811301 |⟩
```

```
1.64146
```

```
7. × 10^19
```

••• FindRoot: The line search decreased the step size to within tolerance specified by AccuracyGoal and PrecisionGoal but was unable to find a sufficient decrease in the merit function. You may need more than MachinePrecision digits of working precision to meet these tolerances.

••• General: Further output of FindRoot::lstol will be suppressed during this calculation.

```
⟨| pmax → 19.4538, vmpp → 0.692, jmpp → -28.1125,
 eff → 0.194538, jsc → 30., voc → 0.821745, ff → 0.789126 |⟩
```

```
1.78963
```

```
8. × 10^19
```

```
⟨| pmax → 17.6658, vmpp → 0.635, jmpp → -27.8202,
 eff → 0.176658, jsc → 30., voc → 0.767553, ff → 0.767191 |⟩
```

```
1.92256
```

```
9. × 10^19
```

```
⟨| pmax → 16.0051, vmpp → 0.582, jmpp → -27.5003,
 eff → 0.160051, jsc → 30., voc → 0.715439, ff → 0.745703 |⟩
```

```
2.03079
```

```
1. × 10^20
```

```
⟨| pmax → 14.4792, vmpp → 0.532, jmpp → -27.2166,
 eff → 0.144792, jsc → 30., voc → 0.665786, ff → 0.72492 |⟩
```

```
2.11313
```