1. (Run this item first) Transmittance I (Ayri-fun. based solution from section “WAVEFUNCTIONS”)

2. Transmittance II (in case when slope of IV region becomes flat, from section “WAVEFUNCTIONS II”, see Appendix)

3. Set of initial parameters: Sample 3 model, Asymmetric AlO/HZO(3nm) + POTENTIAL plotting, w =0.01 (P-induced interfacial charge screening)

```
In[1]:= Tab1ExpData2 = Import["5nm.txt", "Table"]; (*Experimental data input*)
w = 0.01;  (*bias V-induced screening on/off  (w = 1.0 or 0.01) *)
Slp = 2.1;  (* = λL *)
Slrp = 0.6;  (* = λR *)
delta1 = 1.2; (* δ1 = 0.12 nm *)
delta2 = 4.5; (* δ2 = 0.45  nm *)

(*hb=6.58211928*10^(-16) (* Planka Constant [eV s]*);
me=9.10938188`*^-31;
elc=1.602176462*10^(-19);  cp=(2*me/((hb^2)*elc)*10^-20 ); (* 1/(eV*Angstrom^2) *) *)
elc = 1.602176462 * 10^(-19); (* electron charge *)
cp = 0.26246842; (* dimensional coefficient*)
εf = 30.0; (*relative dielectric constant*)
ε0 = (8.85418 * 10^(-12) * 1 / elc) / 10^10  (*  e/(V A) *);
P3 = 10^(-6) * 624.1509;
(*dimensional coeficient μC/cm^2  ==>   F V/m^2 => (* e/(A^2) *)*)
Ps = 12.0; (* Value of sarurated polarization Ps[μC/cm^2]*)
(*  PsVFunc[eV_]:=If[eV<=2.0,Ps,-Ps]; (* Voltage induced P-switching*)    *)
ε1 = (8.85418 * 10^(-12) * 1 / elc) / 10^10;

Fi1 = 0.21;
Fi2 = -0.62;

(*List of effective masses*)
m1 = 0.8 * cp;
m2 = 0.6 * cp;
m3 = 0.4 * cp;
```

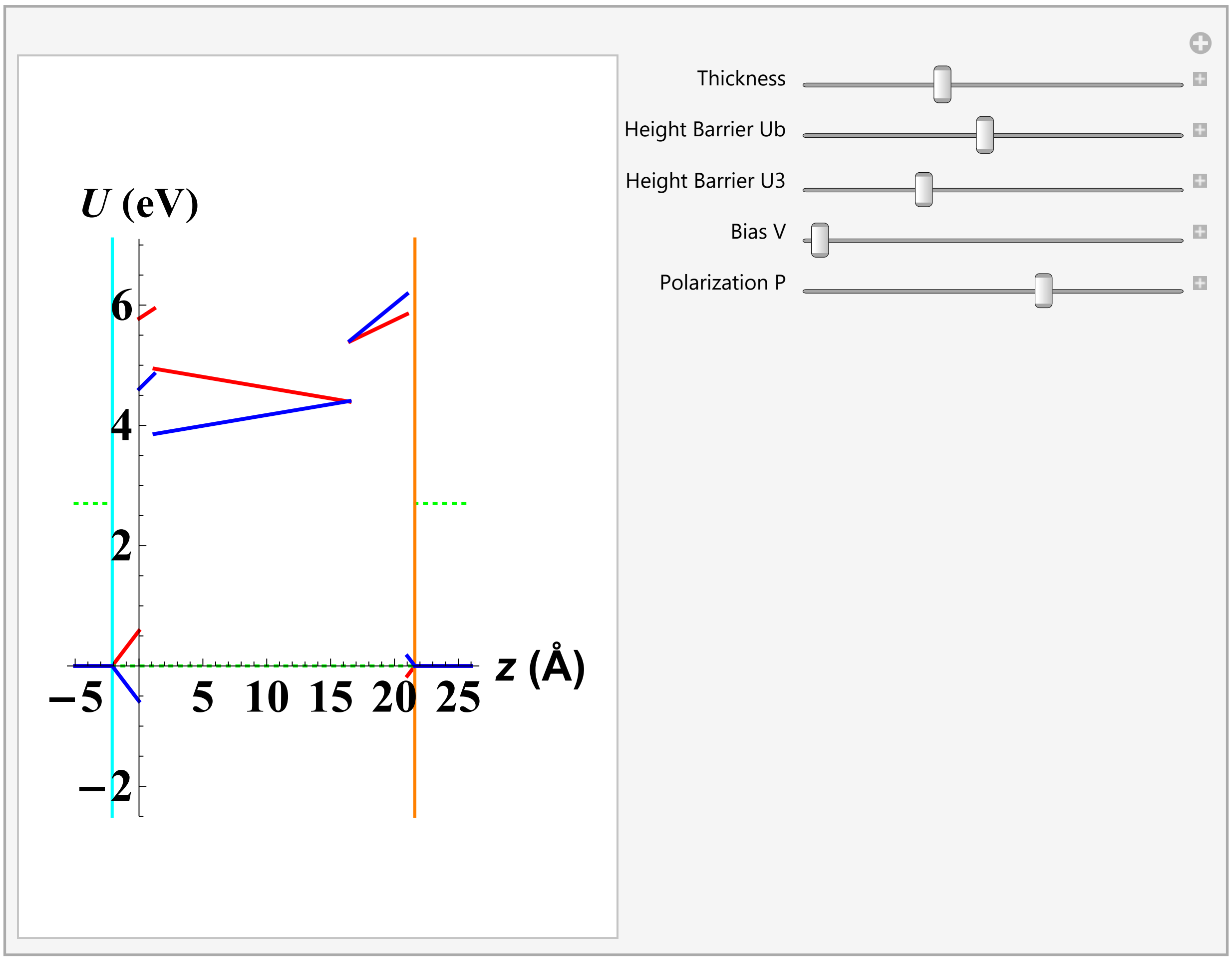
```
m4 = 0.4 * cp;
m5 = 0.4 * cp;
 m6 = 0.6 * cp;
m7 = m1;
(*Fermi level in eV*)
E1p = 2.70;
(*E2p=3.7; *) (*in good metal*)

k1 = Sqrt[m1 * E1p];
k7 = Sqrt[m7 * E1p];

Ubp = E1p + 1.7; (*Barrier Height: Fermi level + the barrier height above*)
U3p = -1.0;      (*Barrier Height regulation of the additional
 barriers inside FE in relation of the edge of the Conduction Band in FE*)

AngleLp = 0.0; (*Due to trnasmission depens from angle,
this value correspond to the perpendicular direction in relation to interface*)
Lp = 15.3 + delta1 + delta2; (* L + δ1 + δ2 *)

(*Parameters for J-V due to Hysteresis see in related section*)

mef[1] = m1;
mef[2] = m2;
mef[3] = m3;
mef[4] = m4;
mef[5] = m5;
mef[6] = m6;
mef[7] = m7;

(*Screeining Charge density*)
ss[P_, eV_, L_, Sl_, Slr_] :=
  L * P * P3 / (ε0 * (L + εf * (Sl + Slr))) + w * εf * eV / (L + εf * (Sl + Slr));

(*Screeining Amplitudes*)
edVm[P_, eV_, L_, x_, Sl_, Slr_] := ss[P, eV, L, Sl, Slr] * x + ss[P, eV, L, Sl, Slr] * Sl;
edV[P_, eV_, L_, x_, Sl_, Slr_] :=
  ss[P, eV, L, Sl, Slr] * x - ss[P, eV, L, Sl, Slr] * (L + Slr) - eV;

y4d1[P_, eV_, L_, Sl_, Slr_, Ub_, U3_] :=
  -(ss[P, eV, L, Sl, Slr] * Sl + ss[P, eV, L, Sl, Slr] * Slr + eV) * delta1 / L +
   Ub - U3 + ss[P, eV, L, Sl, Slr] * Sl;
y4d2[P_, eV_, L_, Sl_, Slr_, Ub_, U3_] :=
  -(ss[P, eV, L, Sl, Slr] * Sl + ss[P, eV, L, Sl, Slr] * Slr + eV) * (L - delta2) / L +
   Ub - U3 + ss[P, eV, L, Sl, Slr] * Sl;
```

In[42]:=
```
VxV2[x_, L_, U2_, eV_, P_, Sl_, Slr_, U3_] := edVm[P, eV, L, x, Sl, Slr] *
     UnitStep[x + Sl] * UnitStep[-x] +
    ((y4d1[P, eV, L, Sl, Slr, U2, U3] - (U2 - U3 + ss[P, eV, L, Sl, Slr] * Sl - Fi1)) * x / delta1 +
       U2 - U3 + ss[P, eV, L, Sl, Slr] * Sl - Fi1) *
     UnitStep[x] * UnitStep[delta1 - x] + (U2 + ss[P, eV, L, Sl,  Slr] * Sl -
       x / L * (eV + ss[P, eV, L, Sl,  Slr] * Sl + ss[P, eV, L, Sl,  Slr] * Slr)) *
     UnitStep[x - delta1] * UnitStep[L - delta2 - x] +
    ((U2 - U3 - ss[P, eV, L, Sl, Slr] * Slr - eV - Fi2 - y4d2[P, eV, L, Sl, Slr, U2, U3]) *
         x / delta2 + 1 / delta2 * (L * y4d2[P, eV, L, Sl, Slr, U2, U3] -
           (L - delta2) * (U2 - U3 - ss[P, eV, L, Sl, Slr] * Slr - eV - Fi2))) *
     UnitStep[x - L + delta2] * UnitStep[L - x] +
    edV[P, eV, L, x, Sl, Slr] * UnitStep[x - L] * UnitStep[Slr - (x - L)] -
    eV * UnitStep[x - L - Slr];
```

In[43]:=
```
FermiShift[x_, eV_, L_] := UnitStep[- (x + Slp)] * E1p + (E1p - eV) UnitStep[(x - Slrp) - L];
```

In[44]:=
```
Manipulate[
 Dynamic[Plot[{VxV2[x, L, U, eV, P, Slp, Slrp, U3], FermiShift[x, eV, L], 1000. * (x + Slp),
    1000. * (x - Slrp - L), VxV2[x, L, U, eV, -P, Slp, Slrp, U3]},
   {x, -5, 26}, PlotRange → {-2.5, 7.1}, FrameStyle → Directive[Black, 24],
   AxesLabel → {Style["z (Å)", Bold, 22, FontFamily → "Arial"], Style["U (eV)", Bold, 22]},
   LabelStyle → Directive[Black, FontFamily → "Times New Roman", Bold],
   TicksStyle → {{Black, Large}, {Black, Large}},
   AxesStyle → Directive[Black, FontSize → 18],
   AspectRatio → 1.4, FormatType → TraditionalForm,
   PlotStyle → {{Red, Thick}, {Green, Dotted}, Cyan, Orange, {Blue, Thick}}]],
 {{L, Lp, "Thickness"}, 5.001, 50},
 {{U, Ubp, "Height Barrier Ub"}, -10, 20}, {{U3, U3p, "Height Barrier U3"}, -10, 20},
 {{eV, 0.00, "Bias V"}, 0.01, 2.5, 0.01},
 {{P, Ps, "Polarization P"}, -41, 41, 10.0}, ControlPlacement → Center]
```

Out[44]=



In[ ]:=
```
edVm[Ps, 0.01, Lp, 0.0, Slp, Slrp] (*screening aplitude from left for positive Ps*)
edV[Ps, 0.01, Lp, Lp, Slp, Slrp] (*screening aplitude from right for positive Ps*)
```

Out[ ]= 0.586026

Out[ ]= -0.177436

In[ ]:=

4. (Main Results calc. I) CurrentDensity for positive P (backward)

In[ ]:=

```
Vmin = 0.11;
Vmax = 1.36;
deltaV = 0.07;
eVshift = 0.0001;
(* It can be for example eVshift=0.11  making a whole voltage shift ;*)

x[2] = 0.0;

DtrFa1[E1p, k1, k7, eVshift + Vmin, Ubp, Lp, Slp, Slrp, Ps, U3p, AngleLp]
DtrFa1[E1p, k1, k7, eVshift + Vmin, Ubp, Lp, Slp, Slrp, -Ps, U3p, AngleLp]
DDtrJoined[E1_, k1_, k7_, eV_, U2_, L_, Sl_, Slr_, P_, U3_, AngleL_] :=
  If[N[Abs[1 / L * (eV + ss[P, eV, L, Sl, Slr] * Sl + ss[P, eV, L, Sl, Slr] * Slr)]] >= 0.001,
   DtrFa1[E1, k1, k7, eV, U2, L, Sl, Slr, P, U3, AngleL],
   DtrFFLa1[E1, k1, k7, eV, U2, L, Sl, Slr, P, U3, AngleL]];

G0 = 7.7481 * 10^(-5); (* 2e^2/h  Conductance quantum in Ohm^-1*)
AngleLThreshold[k1_, k7_, eV_] := Re[ArcSin[(Sqrt[k7^2 + m7 * eV]) / k1]];
(*Lets DEFINE THE CURRENT DENSITY
 follow [A.Useinov,H.-H.Lin,N.Useinov,and L.Tagirov,“Spin-
     resolved electron transport in nanoscale heterojunctions.Theory and applications,”
   Journal of Magnetism and Magnetic Materials,vol.508,p.166729,Aug.2020]
 for details doi:10.1016/j.jmmm.2020.166729 *)
CurrentDensityJ[E1_, k1_, k7_, eV_, U2_, L_, Sl_, Slr_, P_, U3_] :=
 If[Sqrt[k7^2 + m7 * eV] >= k1, Min[k1, k7]^2 * eV * G0 / (2.0 * Pi) * NIntegrate[
    Sin[AngleL] * Cos[AngleL] * DDtrJoined[E1, k1, k7, eV, U2, L, Sl, Slr, P, U3, AngleL],
    {AngleL, 0.0, Pi / 2.0}], Min[k1, k7]^2 * eV * G0 / (2.0 * Pi) * NIntegrate[
    Sin[AngleL] * Cos[AngleL] * DDtrJoined[E1, k1, k7, eV, U2, L, Sl, Slr, P, U3, AngleL],
    {AngleL, 0.0, AngleLThreshold[k1, k7, eV]}]]
```

Out[ ]= 8.1778×10^{-9}

Out[ ]= 7.70342×10^{-8}

In[ ]:=

```
(* Positive P component  of the J-V in  A/cm^2 *)
CurrentDensityTable2Jpos :=
  Table[{eVa, 10^6 * CurrentDensityJ[E1p, k1, k7, eVshift + eVa, Ubp, Lp, Slp, Slrp, Ps, U3p] /
      (10^(-8))}, {eVa, Vmin, Vmax, deltaV}];
Export["CurrentDensityTable2Jpos.dat", CurrentDensityTable2Jpos, "Table"];
```

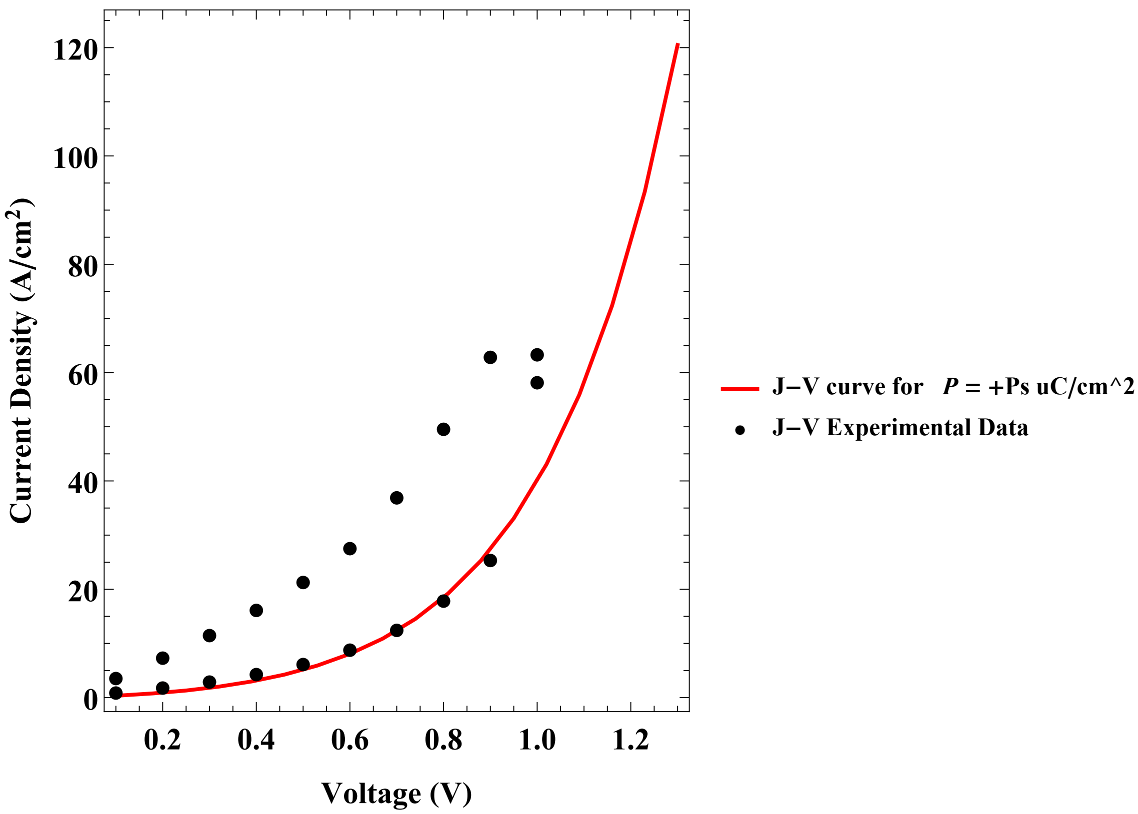
In[ ]:=

```
Tab2pos = Import["CurrentDensityTable2Jpos.dat", "Table"]

{g1, g2} = Graphics /@ {Disk[{0, 0}, 0], Disk[{0, 0}, 1]};


ListPlot[{Tab2pos, Tab1ExpData2}, Joined → {True , False, True} , PlotRange → All,
 PlotStyle → {{Red, Thick}, {Black}, {Orange, Medium}}, AspectRatio → 1.2, Frame → True,
 PlotMarkers → Table[{s, 0.024}, {s, {g1, g2}}],
 TicksStyle → {{Black, Thick}, {Black, Thick}}, FrameStyle → Directive[Black, 16],
 AxesStyle → Directive[Black, FontSize → 15], PlotLegends →
  Placed[{"J-V curve for   P = +Ps uC/cm^2", "J-V Experimental Data"}, Right],
LabelStyle → Directive[Black, FontFamily → "Times New Roman", Bold],
 FrameLabel → {"Voltage (V)", "Current Density (A/cm²)", PlotMarkers → Large}]

ListLogPlot[{Tab2pos, Tab1ExpData2}, Joined → {True , False, True} ,
 PlotRange → All, PlotStyle → {{Red, Thick}, {Black}, {Orange, Medium}},
 AspectRatio → 1.2,
 Frame → True,
 PlotMarkers → Table[{s, 0.024}, {s, {g1, g2}}],
 TicksStyle → {{Black, Thick}, {Black, Thick}},
 FrameStyle → Directive[Black, 16],
 AxesStyle → Directive[Black, FontSize → 15], PlotLegends →
  Placed[{"J-V curve for   P = +Ps uC/cm^2", "J-V Experimental Data"}, Right],
LabelStyle → Directive[Black, FontFamily → "Times New Roman", Bold],
 FrameLabel → {"Voltage (V)", "Current Density (A/cm²)", PlotMarkers → Large}]
```

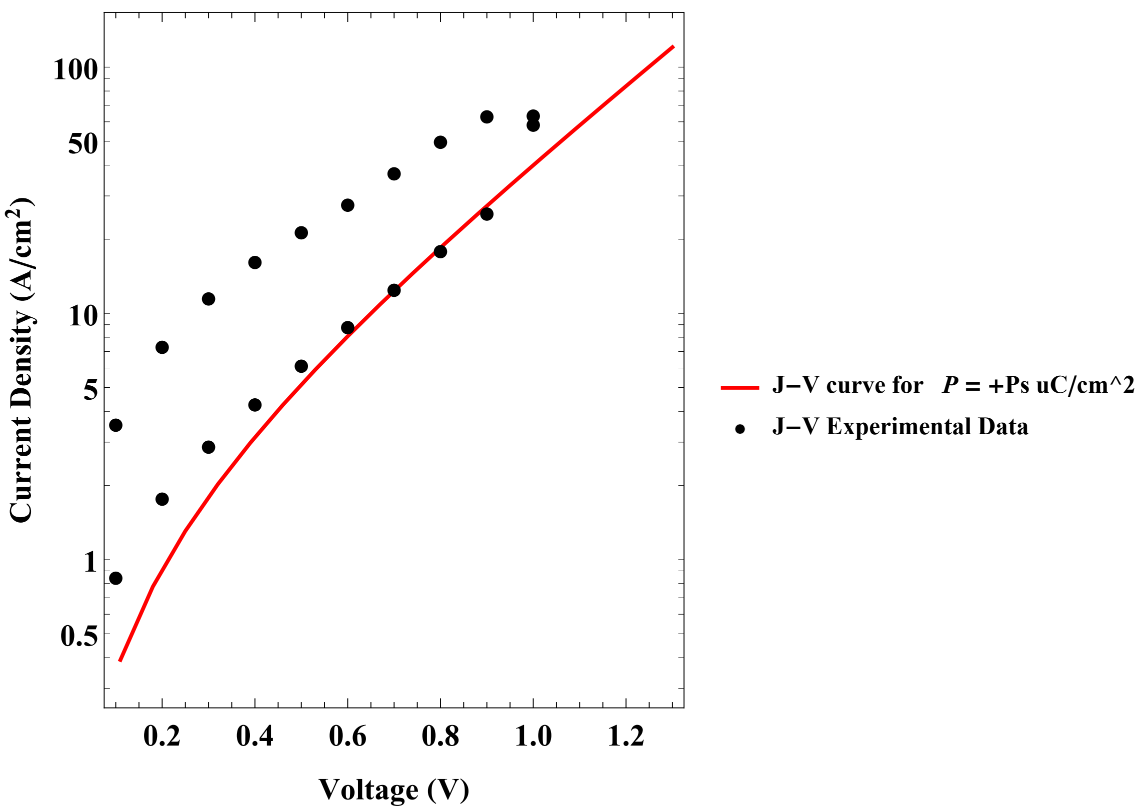
Out[ ]=

```
{{0.11, 0.39158}, {0.18, 0.777209}, {0.25, 1.30695}, {0.32, 2.02294},
 {0.39, 2.97897}, {0.46, 4.24358}, {0.53, 5.9041}, {0.6, 8.07173}, {0.67, 10.8881},
 {0.74, 14.5338}, {0.81, 19.2391}, {0.88, 25.2978}, {0.95, 33.0859},
 {1.02, 43.0841}, {1.09, 55.9096}, {1.16, 72.3548}, {1.23, 93.4407}, {1.3, 120.485}}
```

Out[ ]=


Current Density (A/cm^2)
Voltage (V)
0
20
40
60
80
100
120
0.2
0.4
0.6
0.8
1.0
1.2
J−V curve for P = +Ps uC/cm^2
J−V Experimental Data

Out[ ]=


Current Density (A/cm^2)
Voltage (V)
0.5
1
5
10
50
100
0.2
0.4
0.6
0.8
1.0
1.2
J−V curve for P = +Ps uC/cm^2
J−V Experimental Data

In[ ]:=

5. (Main Results calc. II) CurrentDensity for negative P (forward)

In[∘]:=
```
(* Now calculation of the Negative component by P of the J-V in  A/cm^2,
can be undetermined Integration !!!! *)
CurrentDensityTable1Jneg := Table[
   {eVa, 10^14 * CurrentDensityJ[E1p, k1, k7, eVshift + eVa, Ubp, Lp, Slp, Slrp, -Ps, U3p]},
   {eVa, Vmin, Vmax, deltaV}];  (*in A/cm^2*)
Export["CurrentDensityTable1Jneg.dat", CurrentDensityTable1Jneg, "Table"]
```

NIntegrate: The integrand $1.14019\,\text{Cos[AngleL] Re}\Big[\Big(\text{Sec[AngleL]}\sqrt{1-0.769209\,\text{Sin[≪1≫]}^2}\Big)\Big/\Big(\text{Conjugate[Power[≪2≫] Plus[≪2≫]} + (0. + 4.08862\,i)\,\text{Power[≪2≫] Plus[≪2≫] Power[≪2≫]]}\Big(e^{\text{Times[≪2≫]}}(\text{Times[≪2≫]} + \text{Times[≪2≫]}) + (0. + 4.08862\,i)\,e^{\text{Times[≪2≫]}}(\text{Times[≪2≫]} + \text{Times[≪2≫]})\sqrt{\text{Plus[≪2≫]}}\Big)\Big)\Big]\,\text{Sin[AngleL]}$ has evaluated to Overflow, Indeterminate, or Infinity for all sampling points in the region with boundaries {{0., 1.5708}}.

NIntegrate: The integrand $1.14019\,\text{Cos[AngleL] Re}\Big[\Big(\text{Sec[AngleL]}\sqrt{1-0.769209\,\text{Sin[≪1≫]}^2}\Big)\Big/\Big(\text{Conjugate[Power[≪2≫] Plus[≪2≫]} + (0. + 4.08862\,i)\,\text{Power[≪2≫] Plus[≪2≫] Power[≪2≫]]}\Big(e^{\text{Times[≪2≫]}}(\text{Times[≪2≫]} + \text{Times[≪2≫]}) + (0. + 4.08862\,i)\,e^{\text{Times[≪2≫]}}(\text{Times[≪2≫]} + \text{Times[≪2≫]})\sqrt{\text{Plus[≪2≫]}}\Big)\Big)\Big]\,\text{Sin[AngleL]}$ has evaluated to Overflow, Indeterminate, or Infinity for all sampling points in the region with boundaries {{0., 1.5708}}.

NIntegrate: The integrand $1.14019\,\text{Cos[AngleL] Re}\Big[\Big(\text{Sec[AngleL]}\sqrt{1-0.769209\,\text{Sin[≪1≫]}^2}\Big)\Big/\Big(\text{Conjugate[Power[≪2≫] Plus[≪2≫]} + (0. + 4.08862\,i)\,\text{Power[≪2≫] Plus[≪2≫] Power[≪2≫]]}\Big(e^{\text{Times[≪2≫]}}(\text{Times[≪2≫]} + \text{Times[≪2≫]}) + (0. + 4.08862\,i)\,e^{\text{Times[≪2≫]}}(\text{Times[≪2≫]} + \text{Times[≪2≫]})\sqrt{\text{Plus[≪2≫]}}\Big)\Big)\Big]\,\text{Sin[AngleL]}$ has evaluated to Overflow, Indeterminate, or Infinity for all sampling points in the region with boundaries {{0., 1.5708}}.

General: Further output of NIntegrate::inumri will be suppressed during this calculation.

NIntegrate: Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand, or WorkingPrecision too small.

NIntegrate: NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in AngleL near {AngleL} = {0.536869}. NIntegrate obtained $4.74034\times10^{-7} + 0.\,i$ and 3.955868853023021`*^-12 for the integral and error estimates.

Out[∘]= CurrentDensityTable1Jneg.dat

In[∘]:=
```
(* RE-REATION OF THE NEGATIVE J-
 V CURVE using the knowledge about linear GER behavior and having J-
 V for positive P, which have to be without mistakes!*)
```

In[ ]:=
```
Tab2pos = Import["CurrentDensityTable2Jpos.dat", "Table"]
Tab1b = Import["CurrentDensityTable1Jneg.dat", "Table"]
```

Out[ ]=
```
{{0.11, 0.39158}, {0.18, 0.777209}, {0.25, 1.30695}, {0.32, 2.02294},
 {0.39, 2.97897}, {0.46, 4.24358}, {0.53, 5.9041}, {0.6, 8.07173}, {0.67, 10.8881},
 {0.74, 14.5338}, {0.81, 19.2391}, {0.88, 25.2978}, {0.95, 33.0859},
 {1.02, 43.0841}, {1.09, 55.9096}, {1.16, 72.3548}, {1.23, 93.4407}, {1.3, 120.485}}
```

Out[ ]=
```
{{0.11, 2.62015}, {0.18, 5.23104}, {0.25, 8.86178}, {0.32, 13.8358}, {0.39, 20.5741},
 {0.46, 29.6243}, {0.53, 41.6994}, {0.6, 57.7271}, {0.67, 78.9168}, {0.74, 108.36},
 {0.81, 5.663498490931635*^8*NIntegrate[Sin[AngleL]*Cos[AngleL]*DDtrJoined[2.7,,
  0.7529487281349242,, 0.7529487281349242,, 0.8101,, 4.4,, 21.,,
  2.1,, 0.6,, -12.,, -1.,, AngleL],, {AngleL,, 0.,, Pi/2.}]},
 {0.88, 6.15287621512027*^8*NIntegrate[Sin[AngleL]*Cos[AngleL]*DDtrJoined[2.7,,
  0.7529487281349242,, 0.7529487281349242,, 0.8801,, 4.4,, 21.,,
  2.1,, 0.6,, -12.,, -1.,, AngleL],, {AngleL,, 0.,, Pi/2.}]},
 {0.95, 6.642253939308908*^8*NIntegrate[Sin[AngleL]*Cos[AngleL]*DDtrJoined[2.7,,
  0.7529487281349242,, 0.7529487281349242,, 0.9501000000000001,, 4.4,,
  21.,, 2.1,, 0.6,, -12.,, -1.,, AngleL],, {AngleL,, 0.,, Pi/2.}]},
 {1.02, 338.064}, {1.09, 446.857}, {1.16, 589.627}, {1.23, 777.143}, {1.3, 1023.77}}
```

In[ ]:=
```
(*mistake correction by previous points*)
Tab1c = Table[
  {Tab2pos[[i, 1]], If[NumberQ[Tab1b[[i, 2]]] == False, Tab1b[[i, 2]] = N[Tab2pos[[i, 2]] *
       (2.0 * Tab1b[[i - 1, 2]] / Tab2pos[[i - 1, 2]] - Tab1b[[i - 2, 2]] / Tab2pos[[i - 2, 2]])],
    Tab1b[[i, 2]]]}, {i, 1, Length[Tab2pos]}]

Export["CurrentDensityTable1JnegCor.dat", Tab1c, "Table"];
```

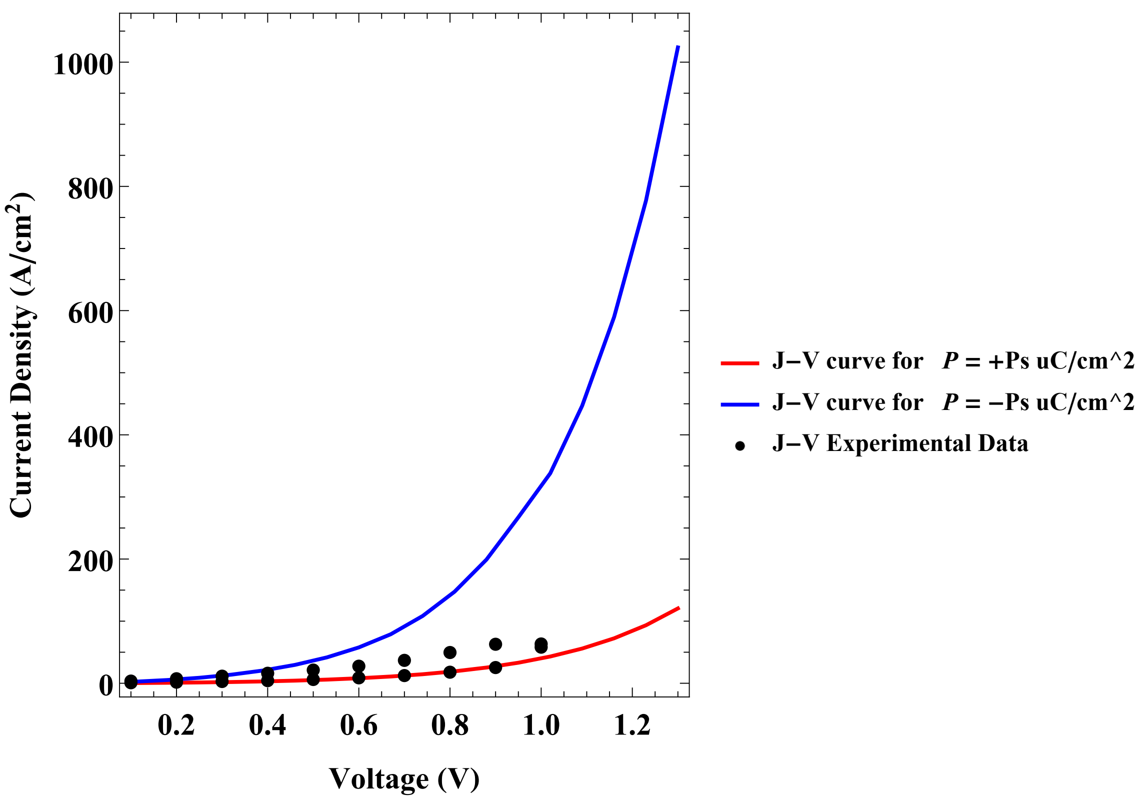
Out[ ]=
```
{{0.11, 2.62015}, {0.18, 5.23104}, {0.25, 8.86178}, {0.32, 13.8358},
 {0.39, 20.5741}, {0.46, 29.6243}, {0.53, 41.6994}, {0.6, 57.7271}, {0.67, 78.9168},
 {0.74, 108.36}, {0.81, 147.438}, {0.88, 199.125}, {0.95, 267.301}, {1.02, 338.064},
 {1.09, 446.857}, {1.16, 589.627}, {1.23, 777.143}, {1.3, 1023.77}}
```

In[ ]:=
```
Tab1neg = Import["CurrentDensityTable1JnegCor.dat", "Table"];
```

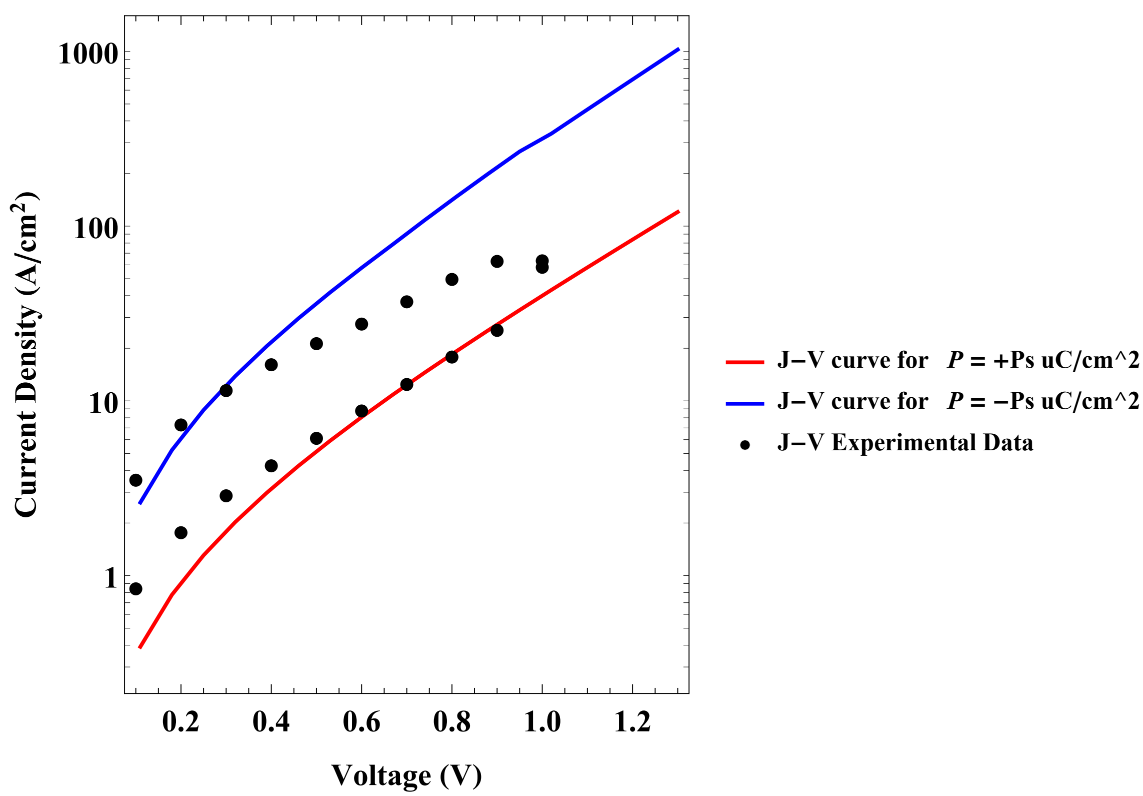
In[ ]:=

```
{g1, g2, g3} = Graphics /@ {Disk[{0, 0}, 0], Disk[{0, 0}, 0], Disk[{0, 0}, 1]};

ListPlot[{Tab2pos, Tab1neg, Tab1ExpData2}, Joined → {True, True , False, True} ,
 PlotRange → All, PlotStyle → {{Red, Thick}, {Blue, Thick}, {Black}, {Orange, Medium}},
 AspectRatio → 1.2, Frame → True, PlotMarkers → Table[{s, 0.024}, {s, {g1, g2, g3}}],
 TicksStyle → {{Black, Thick}, {Black, Thick}}, FrameStyle → Directive[Black, 16],
 AxesStyle → Directive[Black, FontSize → 15], PlotLegends →
  Placed[{"J-V curve for   P = +Ps uC/cm^2", "J-V curve for   P = -Ps uC/cm^2",
    "J-V Experimental Data", "J-V curve Due to Transition P-E"}, Right],
LabelStyle → Directive[Black, FontFamily → "Times New Roman", Bold],
 FrameLabel → {"Voltage (V)", "Current Density (A/cm²)", PlotMarkers → Large}]

ListLogPlot[{Tab2pos, Tab1neg, Tab1ExpData2}, Joined → {True, True , False, True} ,
 PlotRange → All, PlotStyle → {{Red, Thick}, {Blue, Thick}, {Black}, {Orange, Medium}},
 AspectRatio → 1.2, Frame → True, PlotMarkers → Table[{s, 0.024}, {s, {g1, g2, g3}}],
 TicksStyle → {{Black, Thick}, {Black, Thick}}, FrameStyle → Directive[Black, 16],
 AxesStyle → Directive[Black, FontSize → 15], PlotLegends →
  Placed[{"J-V curve for   P = +Ps uC/cm^2", "J-V curve for   P = -Ps uC/cm^2",
    "J-V Experimental Data", "J-V curve Due to Transition P-E"}, Right],
LabelStyle → Directive[Black, FontFamily → "Times New Roman", Bold],
 FrameLabel → {"Voltage (V)", "Current Density (A/cm²)", PlotMarkers → Large}]
```

Out[ ]=



Out[ ]=



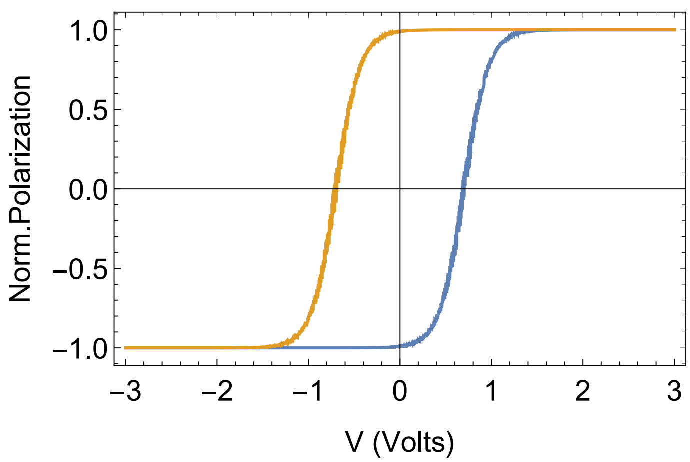
6. J - V calculation due to P - E Hysteresis w=0.01

In[ ]:=

```
(* J-V calculation due to P-E Hysteresis*)

Tab11 = Import["CurrentDensityTable1JnegCor.dat", "Table"];
Tab22 = Import["CurrentDensityTable2Jpos.dat", "Table"];

(* THEN Files  CurrentDensityTable1Jneg.dat HAVE TO BE
 CHEKED AND IMPROVED IF NEEDED if there is integration errors*)

(* Tab1c=Table[{If[NumberQ[Tab1[[i,2]]],  Tab1[[i,1]],0],
   If[NumberQ[Tab1[[i,2]]],Tab1[[i,2]],0]},{i,1,Length[Tab1]}];
Tab2c=Table[{If[NumberQ[Tab2[[i,2]]],  Tab2[[i,1]],0],
   If[NumberQ[Tab2[[i,2]]],Tab2[[i,2]],0]},{i,1,Length[Tab2]}];

Tab3c=
 Table[{Tab1c[[i,1]],If[NumberQ[Tab1[[i,2]]]|| NumberQ[Tab2[[i,2]]],Tab1[[i,2]],0]*
    (Tab1c[[i,2]]*(1-PsVFuncNegtoPosR[1,Tab1c[[i,1]]])+
       Tab2c[[i,2]]*(1+PsVFuncNegtoPosR[1,Tab1c[[i,1]]]))/2.0 },{i,1,Length[Tab1c]}];
Export["CurrentDensityTableHJart.dat",Tab3c,"Table"]; *)
```

In[ ]:=
```
(*Check P-E Hysteresis loop functional dependence,
This function will be aPsled for the J-V due to P-E transoition*)
(*  PsVFunc[eV_]:=If[eV≤1.8,Ps,-Ps];
(* RAPID model of switching - Voltage induced P-switching*)    *)

(* MODEL based on J-V calculation due to P-V Hysteresis*)

Slope = 3.8;
Shift = 0.7;
RandomnessRange = 0.20;    (* Randomness is 20 % as maximum *)

Rm = RandomnessRange / 2.0;

PsVFuncNegtoPos[P_, eV_] := P * Tanh[Slope * (eV - Shift)];
(* Voltage induced P-switching 2 by Tanh  by E-Hysteresis by AFM*)
PsVFuncPostoNeg[P_, eV_] := P * Tanh[Slope * (eV + Shift)];
(* Voltage induced P-switching 2 by Tanh  by E-
 Hysteresis by AFM in case of additional Randomness *)

PsVFuncNegtoPosR[P_, eV_] := P * Tanh[Slope * (eV - Shift)] +
   (1 - Abs[Tanh[Slope * (eV - Shift)]]) * P * RandomReal[{-Rm, Rm}];
PsVFuncPostoNegR[P_, eV_] := P * Tanh[Slope * (eV + Shift)] +
   (1 - Abs[Tanh[Slope * (eV + Shift)]]) * P * RandomReal[{-Rm, Rm}];
Plot[{PsVFuncNegtoPosR[Ps, eV] / Ps, PsVFuncPostoNegR[Ps, eV] / Ps},
 {eV, -3, 3}, Frame → True, FrameStyle → Directive[Black, 15],
 FrameLabel → {"V (Volts)", "Norm.Polarization"}]
```

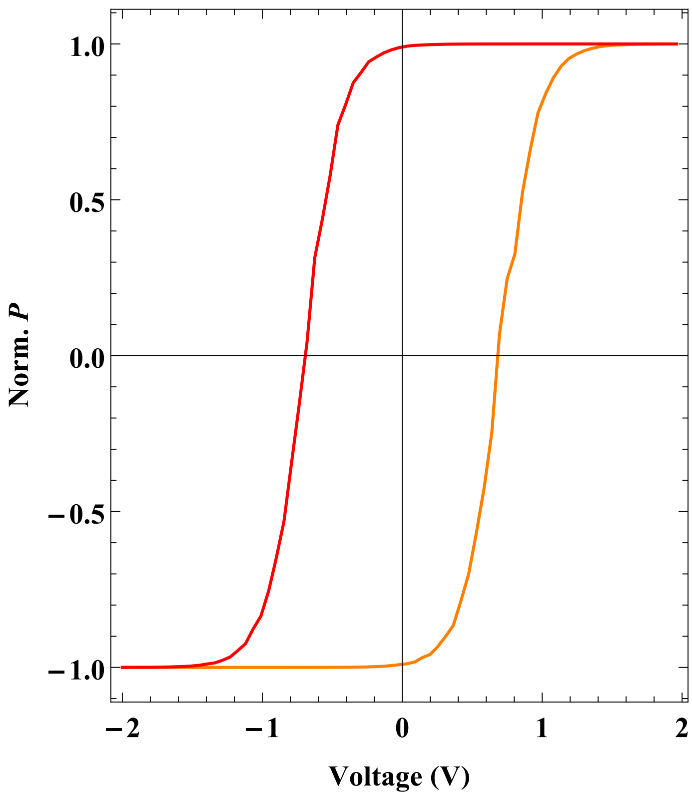
Out[ ]=



```
(* PpVFuncNegtoPosR[P_,eV_]:=If[eV<2.1  && eV>1.8 , P*Tanh[5.0*(eV-2.0)]+
    (1-Abs[Tanh[5.0*(eV-2.0)]])*P*RandomReal[{-0.25,0.25}],P*Tanh[5.0*(eV-2.0)]]; *)
(* PpVFuncNegtoPosR[P_,eV_]:= P*Tanh[5.0*(eV-2.0)]+
   (1-Abs[Tanh[5.0*(eV-2.0)]])*P*RandomReal[{-0.15,0.15}];
PpVFuncPostoNegR[P_,eV_]:= P*Tanh[5.0*(eV+2.0)]+
   (1-Abs[Tanh[5.0*(eV+2.0)]])*P*RandomReal[{-0.15,0.15}];  *)
TG1 = Table[{eV, PsVFuncNegtoPosR[Ps, eV] / Ps}, {eV, -2.0, 2.0, 0.055}];
TG2 = Table[{eV, PsVFuncPostoNegR[Ps, eV] / Ps}, {eV, -2.0, 2.0, 0.055}];
TG3 = Table[{eV, PsVFuncPostoNegR[Ps, eV] / Ps}, {eV, -2.0, 2.0, 0.0015}];
```

In[•]:=
```
ListPlot[{TG1, TG2}, PlotRange → All, Frame → True, FrameStyle → Directive[Black, 15],
 AspectRatio → 1.2, LabelStyle → Directive[Black, FontFamily → "Times New Roman", Bold],
 FrameLabel → {"Voltage (V)", "Norm. P"}, Joined → {True, True}, PlotStyle → {Orange, Red}]
```

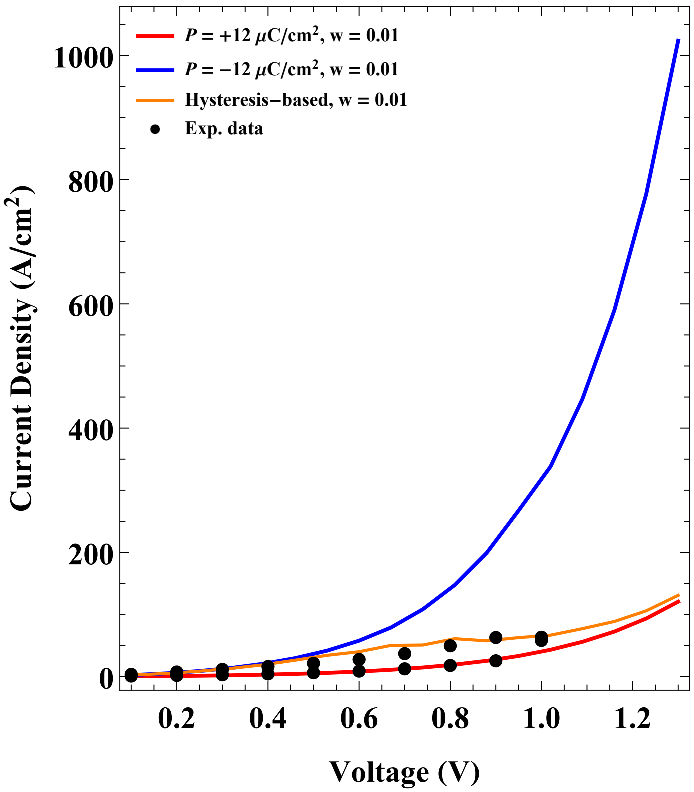
Out[•]=



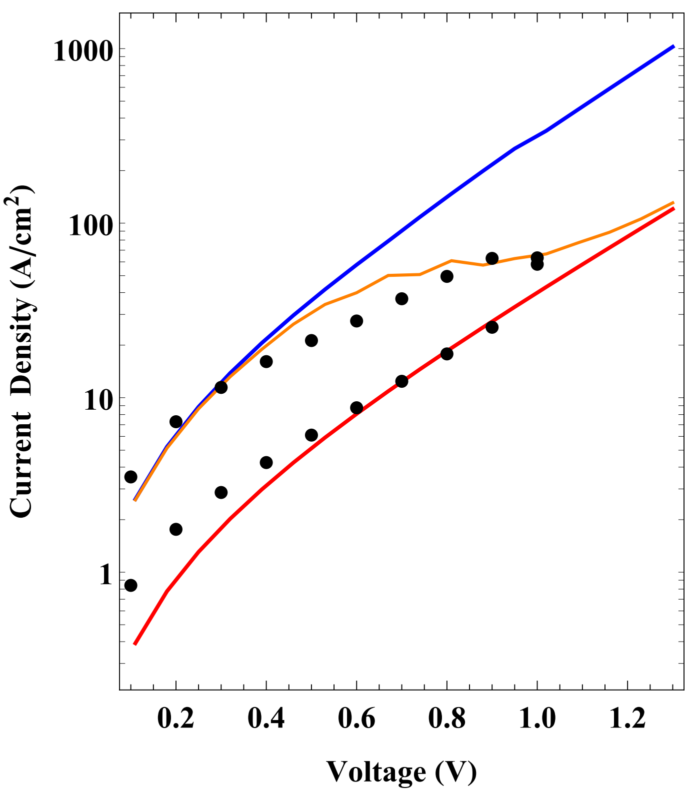
```
Tab31 = Table[
   {Tab11[[i, 1]], (Tab11[[i, 2]] * (1 - PsVFuncNegtoPosR[1, Tab11[[i, 1]]]) + Tab22[[i, 2]] *
        (1 + PsVFuncNegtoPosR[1, Tab11[[i, 1]]])) / 2.0 }, {i, 1, Length[Tab11]}]
Export["CurrentDensityDueToP-E_Hyst.dat", Tab31, "Table"]

{g1, g2, g3, g4} =
  Graphics /@ {Disk[{0, 0}, 0], Disk[{0, 0}, 0], Disk[{0, 0}, 0], Disk[{0, 0}, 1]};

ListPlot[{Tab22, Tab11, Tab31, Tab1ExpData2},
 Joined → {True, True , True, False} , PlotRange → All,
 PlotStyle → {{Red, Thick}, {Blue, Thick}, {Orange, Medium}, {Black}},
 AspectRatio → 1.2,
 Frame → True,
 PlotMarkers → Table[{s, 0.024}, {s, {g1, g2, g3, g4}}],
 TicksStyle → {{Black, Thick}, {Black, Thick}},
 FrameStyle → Directive[Black, 16], AxesStyle → Directive[Black, FontSize → 15],
 AxesStyle → Directive[Black, FontSize → 15],
 PlotLegends → Placed[{"P = +12 μC/cm², w = 0.01", "P = -12 μC/cm², w = 0.01",
    "Hysteresis-based, w = 0.01", "Exp. data" }, {Left, Top}],
LabelStyle → Directive[Black, FontFamily → "Times New Roman", Bold],
 FrameLabel → {"Voltage (V)", "Current Density (A/cm²)", PlotMarkers → Large}]

ListLogPlot[{Tab22, Tab11, Tab31, Tab1ExpData2}, Joined → {True, True , True, False} ,
 PlotRange → All, PlotStyle → {{Red, Thick}, {Blue, Thick}, {Orange, Medium}, {Black}},
 AspectRatio → 1.2,
 Frame → True,
 PlotMarkers → Table[{s, 0.024}, {s, {g1, g2, g3, g4}}],
 TicksStyle → {{Black, Thick}, {Black, Thick}},
 FrameStyle → Directive[Black, 16], AxesStyle → Directive[Black, FontSize → 15],
 AxesStyle → Directive[Black, FontSize → 15],
LabelStyle → Directive[Black, FontFamily → "Times New Roman", Bold],
 FrameLabel → {"Voltage (V)", "Current  Density (A/cm²)", PlotMarkers → Large}]
```

```
Out[•]= {{0.11, 2.59776}, {0.18, 5.13792}, {0.25, 8.64051}, {0.32, 13.1819},
  {0.39, 18.9242}, {0.46, 26.3528}, {0.53, 34.2027}, {0.6, 39.9267}, {0.67, 50.1498},
  {0.74, 50.7499}, {0.81, 60.9067}, {0.88, 57.4731}, {0.95, 62.6649},
  {1.02, 66.6}, {1.09, 77.0832}, {1.16, 88.6499}, {1.23, 105.809}, {1.3, 130.71}}

Out[•]= CurrentDensityDueToP-E_Hyst.dat

Out[•]= {{0.11, 0.0667428}, {0.285, 0.353946}, {0.46, 1.13178},
  {0.635, 2.79921}, {0.81, 6.175}, {0.985, 9.98312}, {1.16, 19.6468}}
```

Out[ ]=



Out[ ]=



7. TER & GER Calculation

In[ ]:=

```
TabTER = Table[{Tab11[[i, 1]], (Tab11[[i, 2]] - Tab22[[i, 2]]) / Tab22[[i, 2]] * 100},
    {i, 1, Length[Tab11]}];
Export["TER_Asym_FTJ2.dat", TabTER, "Table"];

TabGER = Table[{Tab11[[i, 1]], (Tab11[[i, 2]]) / Tab22[[i, 2]]}, {i, 1, Length[Tab11]}]
Export["GER_Asym_FTJ2.dat", TabTER, "Table"];
```

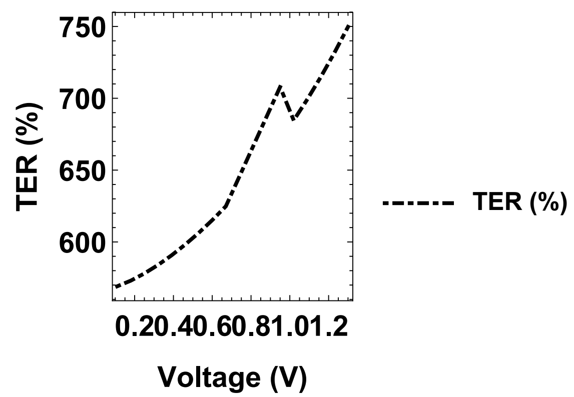
Out[ ]=

```
{{0.11, 6.69122}, {0.18, 6.73054}, {0.25, 6.7805}, {0.32, 6.83945},
 {0.39, 6.90645}, {0.46, 6.98098}, {0.53, 7.06278}, {0.6, 7.15176},
 {0.67, 7.24796}, {0.74, 7.45572}, {0.81, 7.66348}, {0.88, 7.87124}, {0.95, 8.079},
 {1.02, 7.84659}, {1.09, 7.99249}, {1.16, 8.1491}, {1.23, 8.31696}, {1.3, 8.49711}}
```

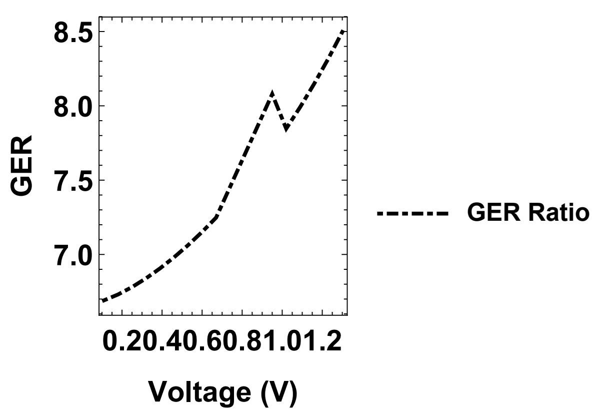
In[ ]:=

```
{ListPlot[{TabTER}, Joined → True, PlotRange → All,
  PlotStyle → { {Black, Thick, DotDashed}}, AspectRatio → 1.2, Frame → True,
  FrameStyle → Directive[Black, 15], PlotLegends → Placed[{"TER (%) "}, Right],
LabelStyle → Directive[Black, Bold], FrameLabel → {"Voltage (V)", "TER (%)"}],
 ListPlot[{TabGER}, Joined → True, PlotRange → All,
  PlotStyle → { {Black, Thick, DotDashed}}, AspectRatio → 1.2, Frame → True,
  FrameStyle → Directive[Black, 15], PlotLegends → Placed[{"GER Ratio"}, Right],
LabelStyle → Directive[Black, Bold], FrameLabel → {"Voltage (V)", "GER"}]}
```

Out[ ]= {



,



}

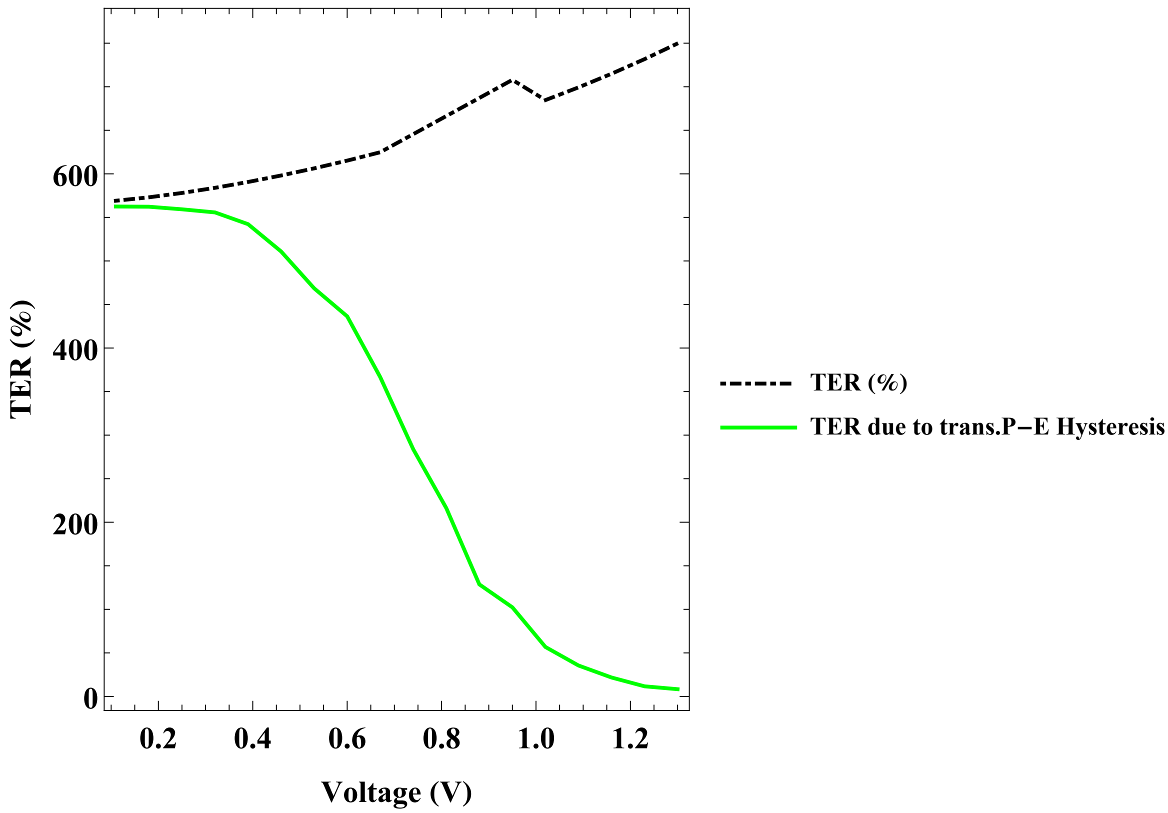
In[ ]:=

```
TabTER2 = Table[{Tab11[[i, 1]], (Tab31[[i, 2]] - Tab22[[i, 2]]) / Tab22[[i, 2]] * 100},
   {i, 1, Length[Tab11]}];
Export["TER_due_to_P-E_Asym_FTJ2.dat", TabTER2, "Table"];
```

In[ ]:=

```
ListPlot[{TabTER, TabTER2}, Joined → True, PlotRange → All,
 PlotStyle → { { Black, Thick, DotDashed}, {Green, Thick}},
 AspectRatio → 1.2,
 FrameStyle → Directive[Black, 16],
 AxesStyle → Directive[Black, FontSize → 15],
 Frame → True, FrameStyle → Directive[Black, 15],
 PlotLegends → Placed[{"TER (%)", "TER due to trans.P-E Hysteresis"}, Right],
LabelStyle → Directive[Black, FontFamily → "Times New Roman", Bold],
 FrameLabel → {"Voltage (V)", "TER (%)"}]
```

Out[ ]=



In[ ]:=

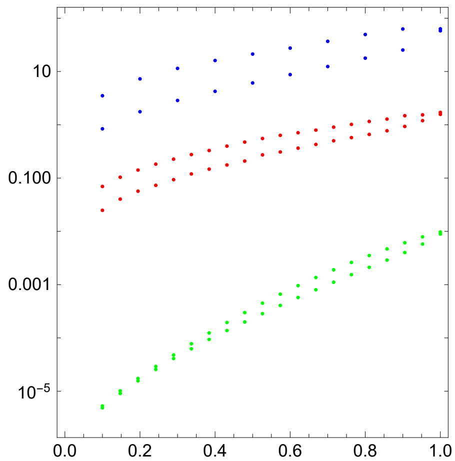
(APsendix I) J-V Exp. Data (M1/IL/HZO(3nm)/Al2O3 (1.4)/M2 & M1/HZO(3nm-4nm)/M2)

In[ ]:=

In[ ]:=
```
Tab1ExpData2 = Import["5nm.txt", "Table"];
Tab1ExpData1 = Import["3nm.txt", "Table"];
Tab1ExpData3 = Import["4nm.txt", "Table"];
```

In[ ]:=
```
ListLogPlot[{Tab1ExpData1, Tab1ExpData2, Tab1ExpData3},
 PlotStyle → {Red, Blue, Green}, AspectRatio → 1.1, Frame → True]
```

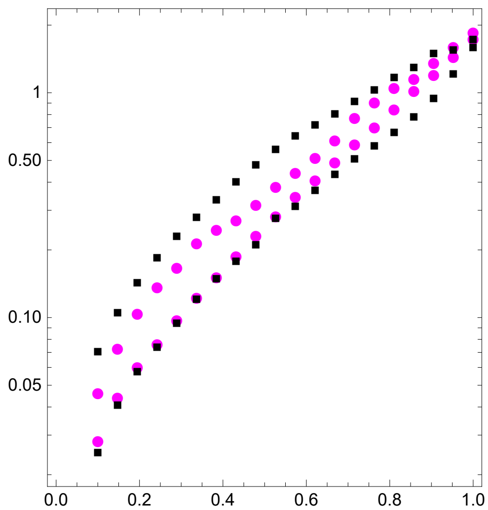
Out[ ]=



In[ ]:=
```
Tab1ExpData4 = Import["3nm_negativeVbranch.txt", "Table"]
ListLogPlot[{Tab1ExpData4, Tab1ExpData1}, PlotStyle → {{Magenta}, {Black}},
 PlotMarkers → {●, ■}, Frame → True, AspectRatio → 1.1]
```

Out[ ]=
```
{{0.1, 0.04609}, {0.14737, 0.07269}, {0.19474, 0.10388}, {0.24211, 0.1365},
 {0.28947, 0.16641}, {0.33684, 0.214}, {0.38421, 0.2458}, {0.43158, 0.27108},
 {0.47895, 0.31669}, {0.52632, 0.38181}, {0.57368, 0.43889}, {0.62105, 0.51316},
 {0.66842, 0.61361}, {0.71579, 0.77181}, {0.76316, 0.90345}, {0.81053, 1.04798},
 {0.85789, 1.15194}, {0.90526, 1.35728}, {0.95263, 1.59984}, {1, 1.85344},
 {1, 1.73031}, {0.95263, 1.44245}, {0.90526, 1.20027}, {0.85789, 1.01502},
 {0.81053, 0.84162}, {0.76316, 0.70153}, {0.71579, 0.58945}, {0.66842, 0.48866},
 {0.62105, 0.40784}, {0.57368, 0.34317}, {0.52632, 0.28142}, {0.47895, 0.23117},
 {0.43158, 0.18725}, {0.38421, 0.15125}, {0.33684, 0.12236}, {0.28947, 0.09735},
 {0.24211, 0.07592}, {0.19474, 0.05998}, {0.14737, 0.044}, {0.1, 0.02815}}
```

Out[ ]=



(APsendix II - WAVEFUNCTIONS) How Wave Functions were derived

(APsendix III, WAVEFUNCTIONS-II) How Wave Functions were derived for simplified flat barrier