HASPIDE – WP3
Simulations (TCAD)
Status Report

04/10/2022

- Charge Transport and Carriers Mobility Models
- An extensive acvitity has been devoted to the modeling of the charge transport within the a-Si:H, relying on standard transport equations for monocrystlline silicon - drift-diffusion (DD) approximation and using a custom defined charge mobility, looking at the current-voltage responses at different temperatures.

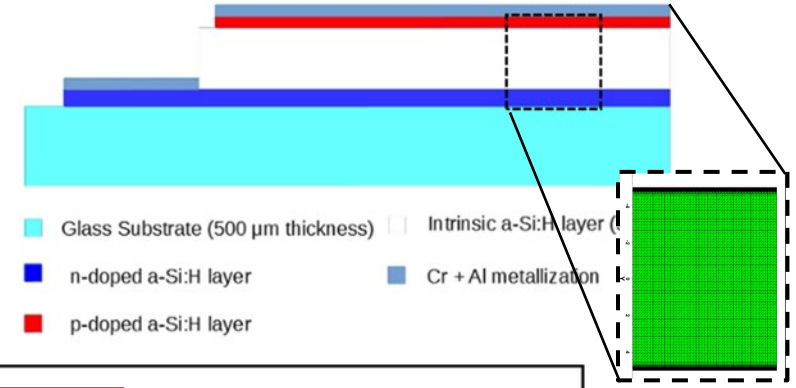
Embedded Transport Models
(DD, TD, HD)

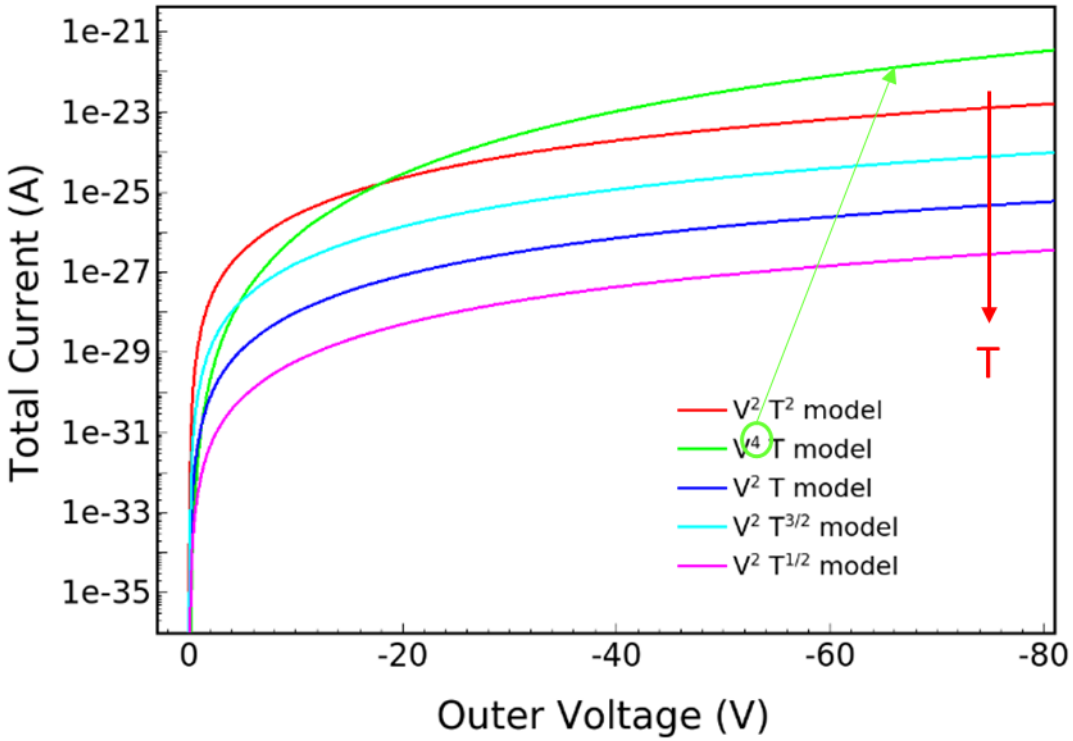
$$\Delta T \rightarrow \Delta\mu \rightarrow \Delta I$$

Custom mobility model
(PMI)

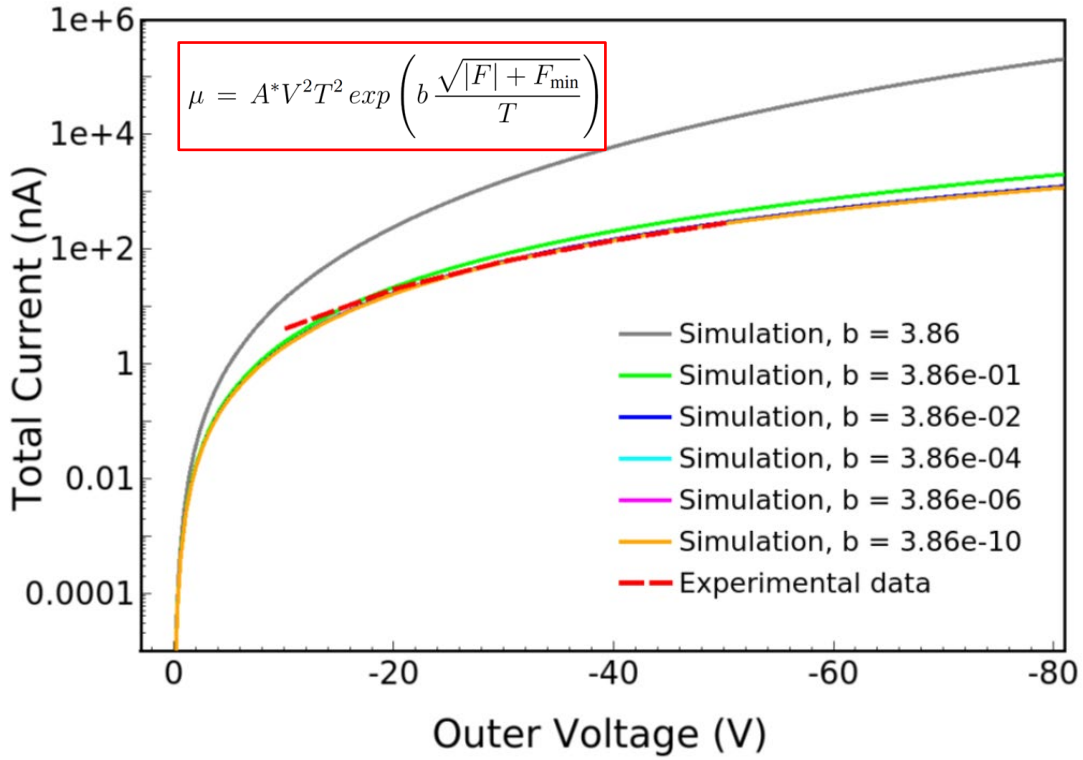
$$\mu = A^* V^2 T^2 exp\left(b \frac{\sqrt{|F| + F_{\min}}}{T}\right)$$

- Model validation: Simulations vs. Measuremens (I-V)
- The effects of changing the exponents of V and T have been studied.





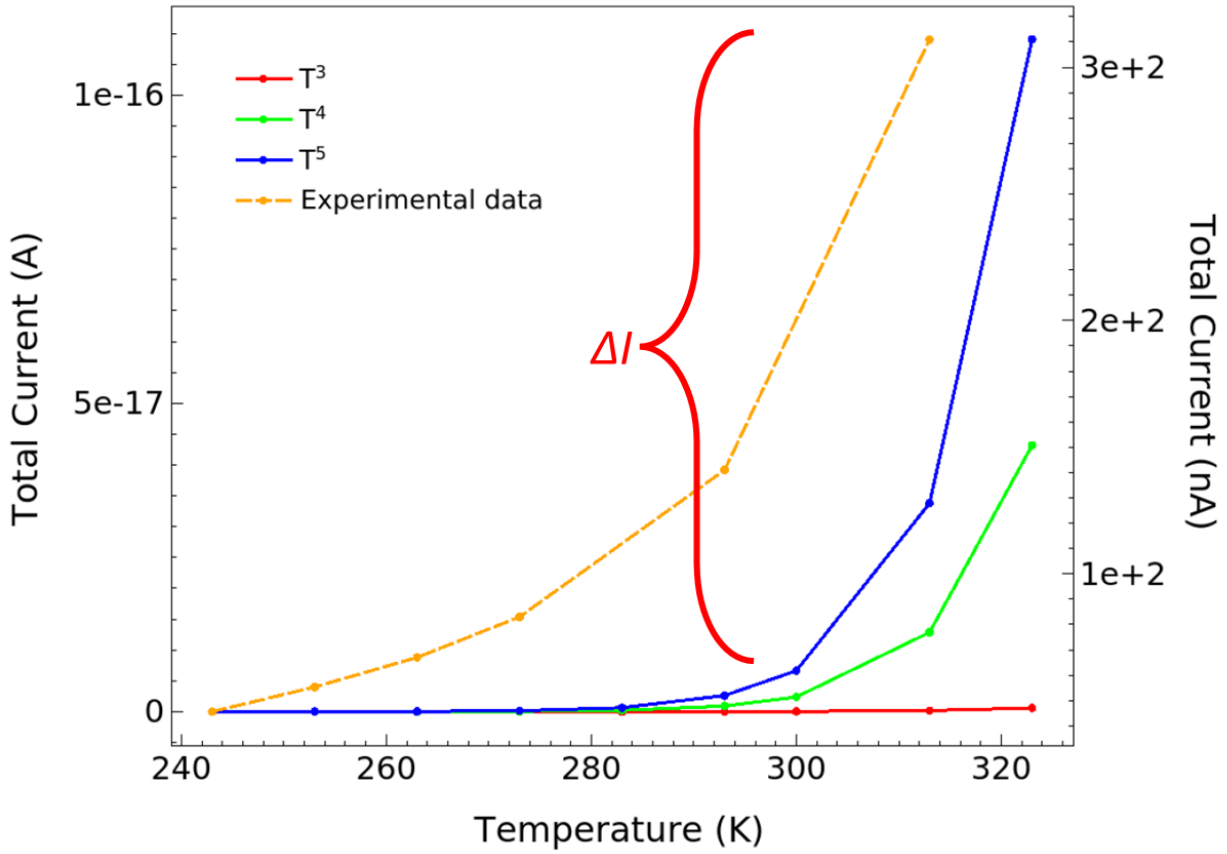
Current vs. Voltage Simulations @ mobilities models



Current vs. Voltage Simulations vs. Measurements

Model validation: focus on T^5 model

- The model with T^5 gives us the best results in terms of ΔI



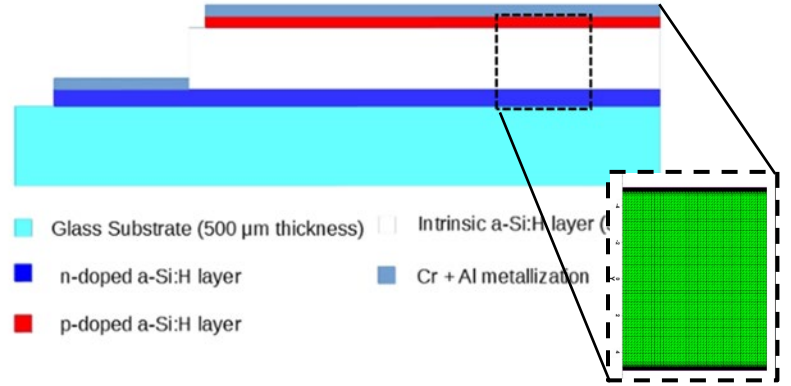
WP3

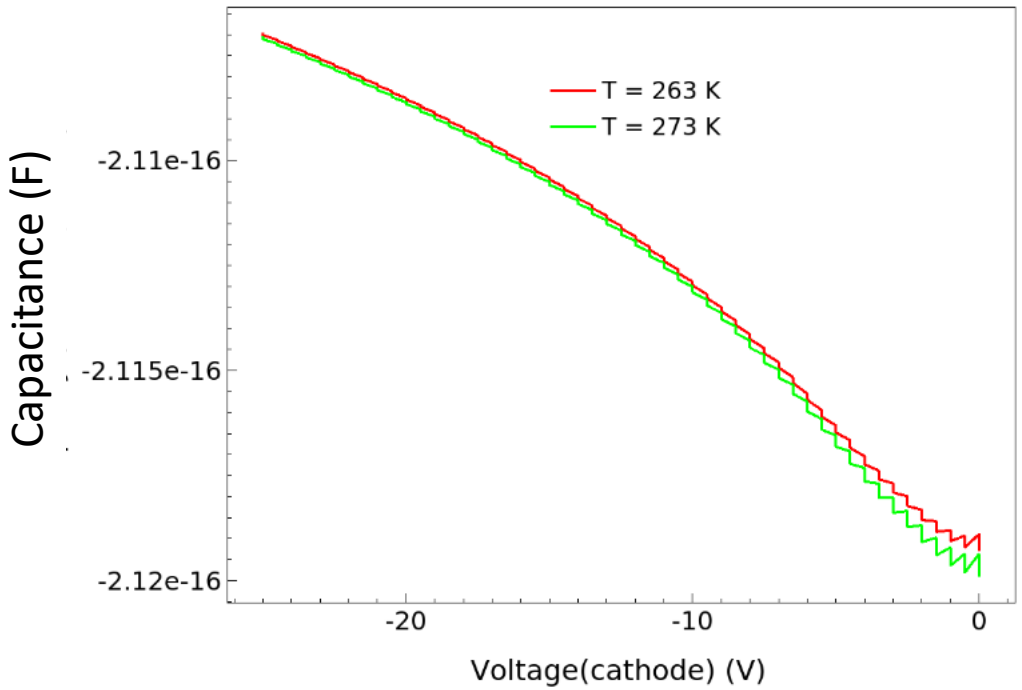
- Capacitance-Voltage simulations:
  - small-signal analyses
  - comparison with measurements.
- a:Si-H: band-gap re-engineering (trap definition $\rightarrow$ single equivalent donor/acceptor modelling).

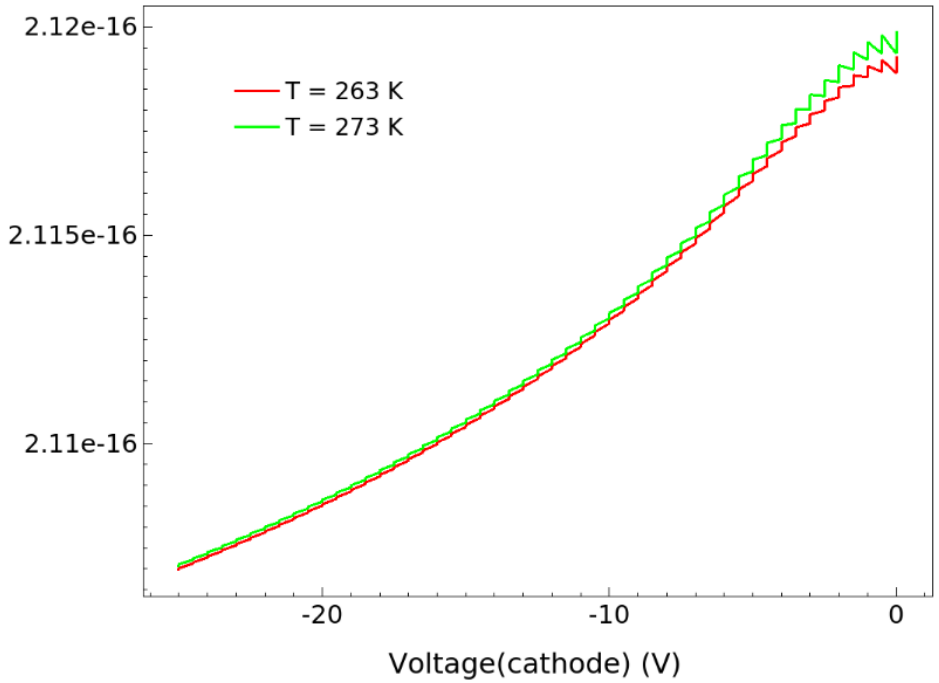
- Capacitance-Voltage simulations

```
151         ACCoupled (
152                 StartFrequency=1e5 EndFrequency=1e6 NumberOfPoints=4 Decade
153                 ACCompute (Time = (Range = (0 0.25) Intervals=50))
154                 Node(cathode anode)
155                 ){ Poisson Electron Hole}
156         }
157
158         Save(FilePrefix="n@node@_quasistationary_Bias-@Bias@V")
```

$$\mu = A^* V^2 T^5 exp\left(b\frac{\sqrt{|F| + F_{min}}}{T}\right)$$





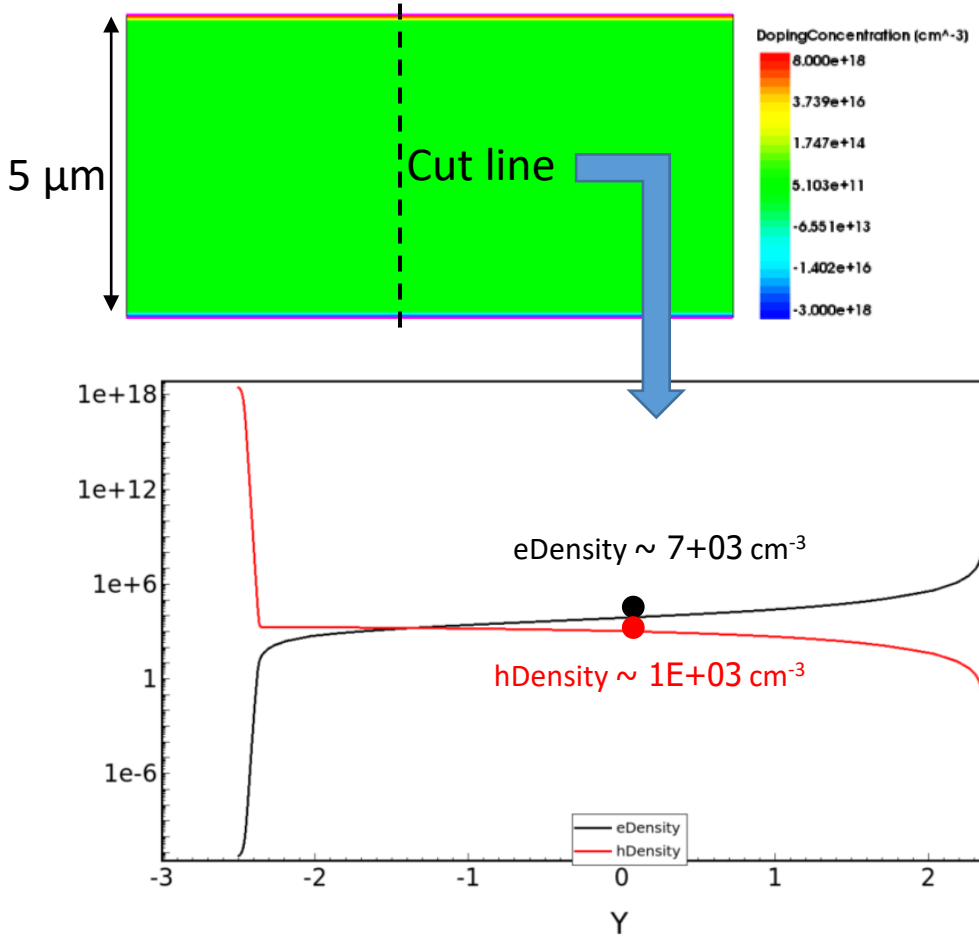


• a-Si:H.par: band-gap description

```
Physics{¶
    Temperature=@<VAR_Temp>@¶
    Recombination(SRH(-DopingDependence)-TrapAssistedAuger)¶
    EffectiveIntrinsicDensity(Bennett)¶
    }¶
¶
Physics{Material="aSiH"}¶
    {¶
----------Mobility(    eHighFieldSaturation-(@ePMI@-@DrivingForce@)¶
                        hHighFieldSaturation-(@hPMI@-@DrivingForce@)¶
----------¶
----------)¶
    Traps(¶
    ----#-Tail-for-Acceptor¶
    ----(Acceptor-Level-EnergyMid=0.04-fromCondBand¶
    ----Conc=--@<8.38e20*AcclntroFac>@--eXsection=1e-16-hXsection=1e-14-
Add2TotalDoping)¶
    ----(Acceptor-Level-EnergyMid=0.19-fromCondBand¶
    ----Conc=--@<7.40e17*AcclntroFac>@--eXsection=1e-16-hXsection=1e-14-
Add2TotalDoping)¶
    ----(Acceptor-Level-EnergyMid=0.34-fromCondBand¶
    ----Conc=--@<4.77e14*AcclntroFac>@--eXsection=1e-16-hXsection=1e-14-
Add2TotalDoping)¶
    ----(Acceptor-Level-EnergyMid=0.49-fromCondBand¶
    ----Conc=--@<3.22e11*AcclntroFac>@--eXsection=1e-16-hXsection=1e-14-
Add2TotalDoping)¶
¶
    ----#-Gaussian-distribution-of-Acceptor-defects¶
    ----(Acceptor-Level-EnergyMid=1.09-fromCondBand¶
    ----Conc=--@<2.00e10*AccConc>@--eXsection=1e-16-hXsection=1e-14-
Add2TotalDoping)¶
    ----(Acceptor-Level-EnergyMid=0.94-fromCondBand¶
    ----Conc=--@<7.02e12*AccConc>@--eXsection=1e-16-hXsection=1e-14-
Add2TotalDoping)¶
    ----(Acceptor-Level-EnergyMid=0.79-fromCondBand¶
    ----Conc=--@<3.10e14*AccConc>@--eXsection=1e-16-hXsection=1e-14-
Add2TotalDoping)¶
    ----(Acceptor-Level-EnergyMid=0.64-fromCondBand¶
    ----Conc=--@<1.09e15*AccConc>@--eXsection=1e-16-hXsection=1e-14-
Add2TotalDoping)¶
    ----(Acceptor-Level-EnergyMid=0.49-fromCondBand¶
    ----Conc=--@<5.08e14*AccConc>@--eXsection=1e-16-hXsection=1e-14-
Add2TotalDoping)¶
    ----(Acceptor-Level-EnergyMid=0.34-fromCondBand¶
    ----Conc=--@<2.37e13*AccConc>@--eXsection=1e-16-hXsection=1e-14-
Add2TotalDoping)¶
    ----(Acceptor-Level-EnergyMid=0.19-fromCondBand¶
    ----Conc=--@<1.16e11*AccConc>@--eXsection=1e-16-hXsection=1e-14-
Add2TotalDoping)¶
¶
    ----#-Gaussian-distribution-of-Donor-defects¶
    ----(Donor-Level-EnergyMid=0.30-fromValBand¶
    ----Conc=--@<1.16e11*DonConc>@--eXsection=1e-14-hXsection=1e-16-
Add2TotalDoping)¶
    ----(Donor-Level-EnergyMid=0.45-fromValBand¶
    ----Conc=--@<2.59e13*DonConc>@--eXsection=1e-14-hXsection=1e-16-
Add2TotalDoping)¶
    ----(Donor-Level-EnergyMid=0.60-fromValBand¶
    ----Conc=--@<5.56e14*DonConc>@--eXsection=1e-14-hXsection=1e-16-
Add2TotalDoping)¶
    ----(Donor-Level-EnergyMid=0.75-fromValBand¶
    ----Conc=--@<1.14e15*DonConc>@--eXsection=1e-14-hXsection=1e-16-
Add2TotalDoping)¶
    ----(Donor-Level-EnergyMid=0.89-fromValBand¶
    ----Conc=--@<3.24e14*DonConc>@--eXsection=1e-14-hXsection=1e-16-
Add2TotalDoping)¶
    ----(Donor-Level-EnergyMid=1.05-fromValBand¶
    ----Conc=--@<8.04e12*DonConc>@--eXsection=1e-14-hXsection=1e-16-
Add2TotalDoping)¶
    ----(Donor-Level-EnergyMid=1.20-fromValBand¶
    ----Conc=--@<3.00e10*DonConc>@--eXsection=1e-14-hXsection=1e-16-
Add2TotalDoping)¶
¶
    ----#-Tail-for-Donor¶
    ----(Donor-Level-EnergyMid=0.00-fromValBand¶
    ----Conc=--@<8.77e20*DonIntroFac>@--eXsection=1e-14-hXsection=1e-16-
Add2TotalDoping)¶
    ----(Donor-Level-EnergyMid=0.15-fromValBand¶
    ----Conc=--@<4.09e19*DonIntroFac>@--eXsection=1e-14-hXsection=1e-16-
Add2TotalDoping)¶
    ----(Donor-Level-EnergyMid=0.30-fromValBand¶
    ----Conc=--@<1.67e18*DonIntroFac>@--eXsection=1e-14-hXsection=1e-16-
Add2TotalDoping)¶
    ----(Donor-Level-EnergyMid=0.45-fromValBand¶
    ----Conc=--@<7.10e16*DonIntroFac>@--eXsection=1e-14-hXsection=1e-16-
Add2TotalDoping)¶
    ----(Donor-Level-EnergyMid=0.59-fromValBand¶
    ----Conc=--@<3.17e15*DonIntroFac>@--eXsection=1e-14-hXsection=1e-16-
Add2TotalDoping)¶
    ----(Donor-Level-EnergyMid=0.75-fromValBand¶
    ----Conc=--@<1.18e14*DonIntroFac>@--eXsection=1e-14-hXsection=1e-16-
Add2TotalDoping)¶
    ----(Donor-Level-EnergyMid=0.90-fromValBand¶
    ----Conc=--@<4.81e12*DonIntroFac>@--eXsection=1e-14-hXsection=1e-16-
Add2TotalDoping)  ¶
    ----(Donor-Level-EnergyMid=1.05-fromValBand¶
    ----Conc=--@<1.96e11*DonIntroFac>@--eXsection=1e-14-hXsection=1e-16-
Add2TotalDoping)  -¶
    ----)  ¶
    }  ¶
¶
)¶
```

• a-Si:H.par: band-gap description (2)

Simulated Layout

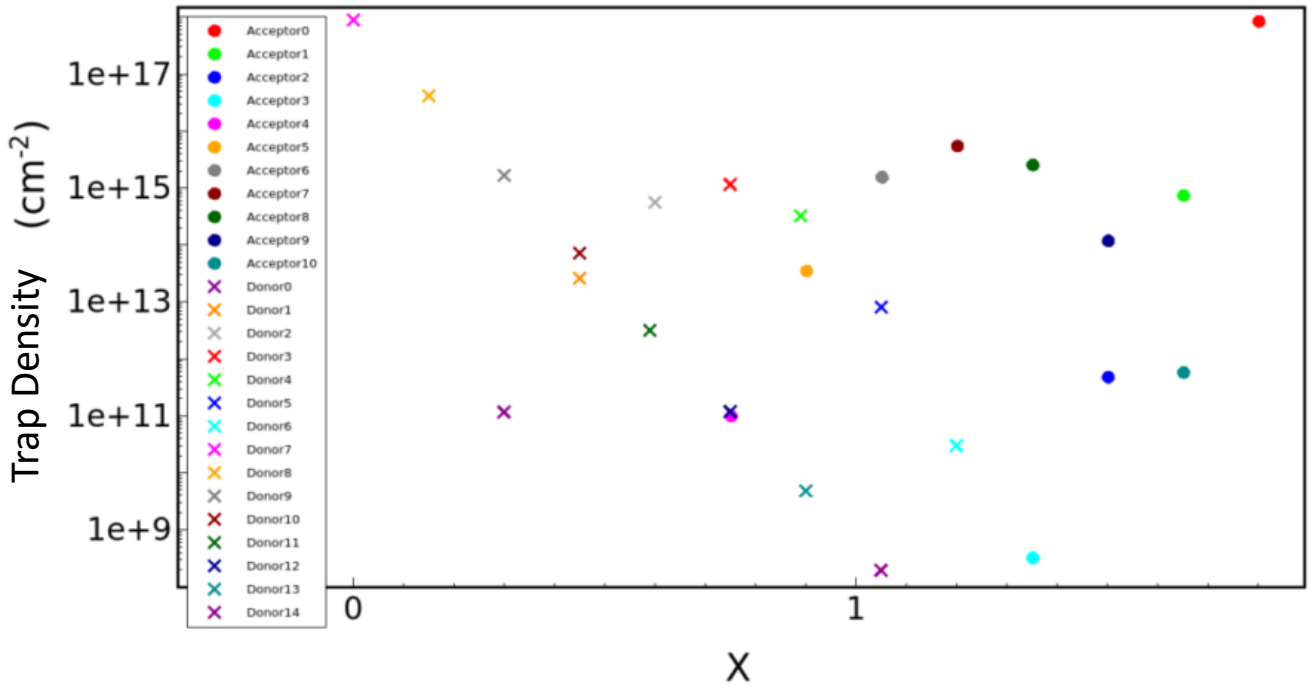


INPUT to TCAD:

Acceptor ●

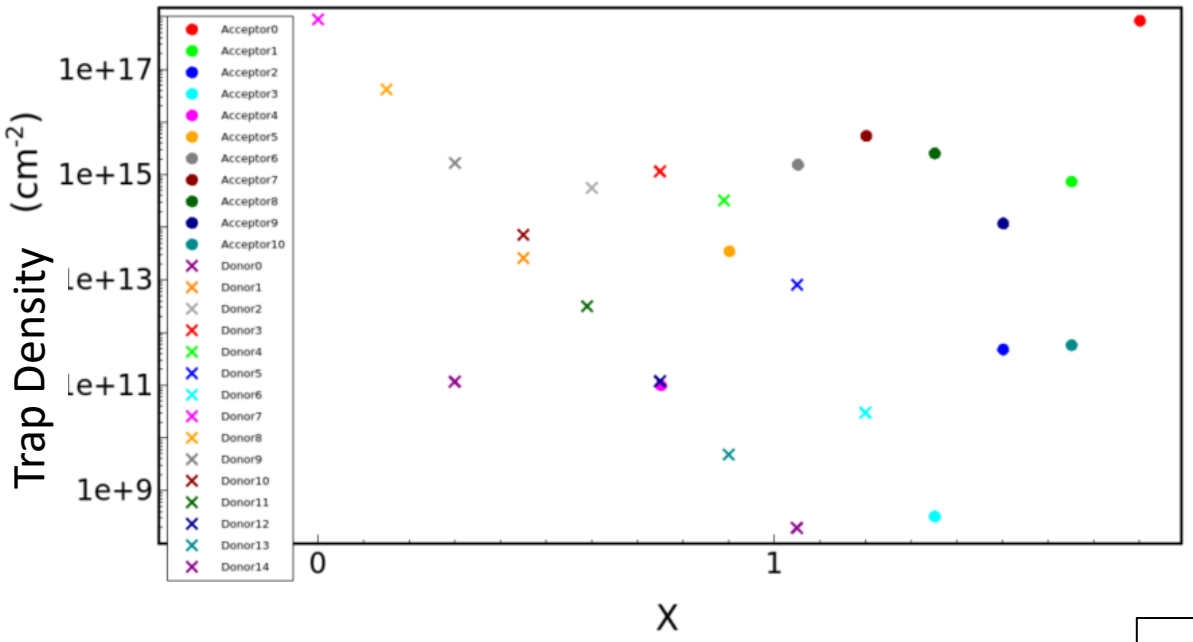
Donor X

Trap Density

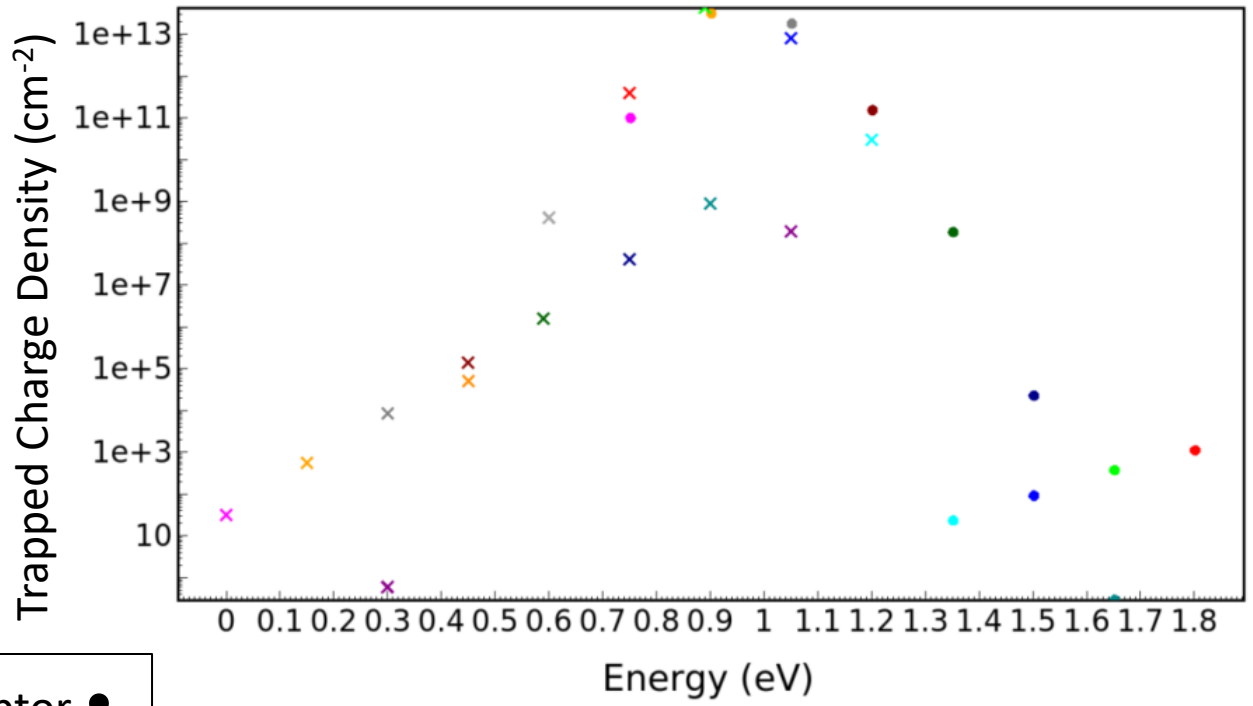


- a-Si:H.par: band-gap description (3)

INPUT to TCAD:



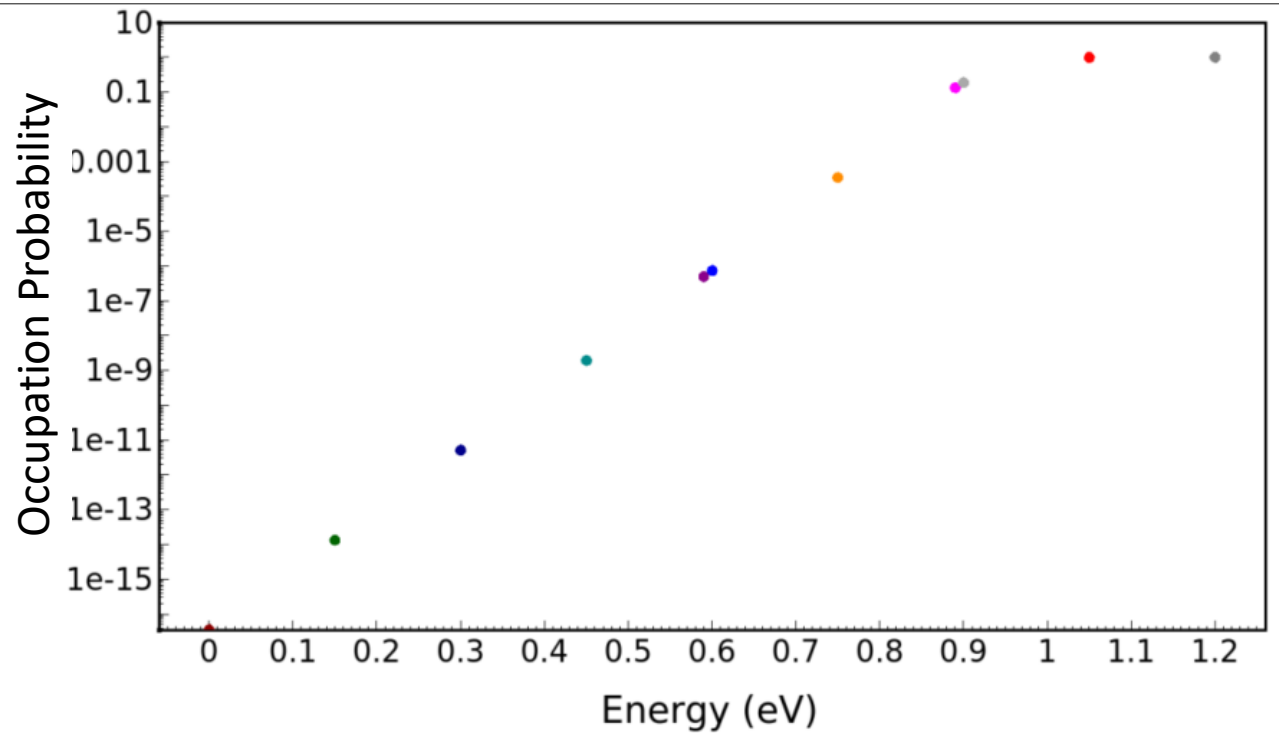
OUTPUT of the device simulation:



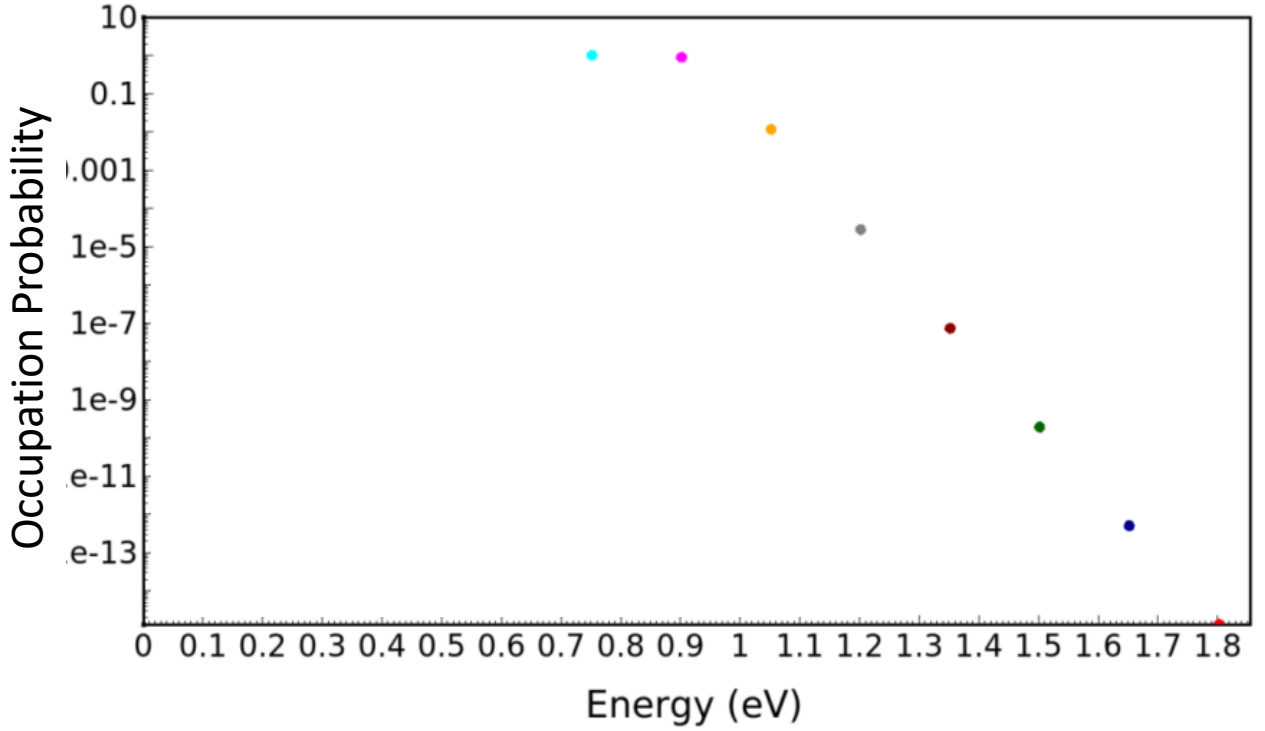
Acceptor ●
Donor X

- a-Si:H.par: band-gap description (4)

DONOR



ACCEPTOR

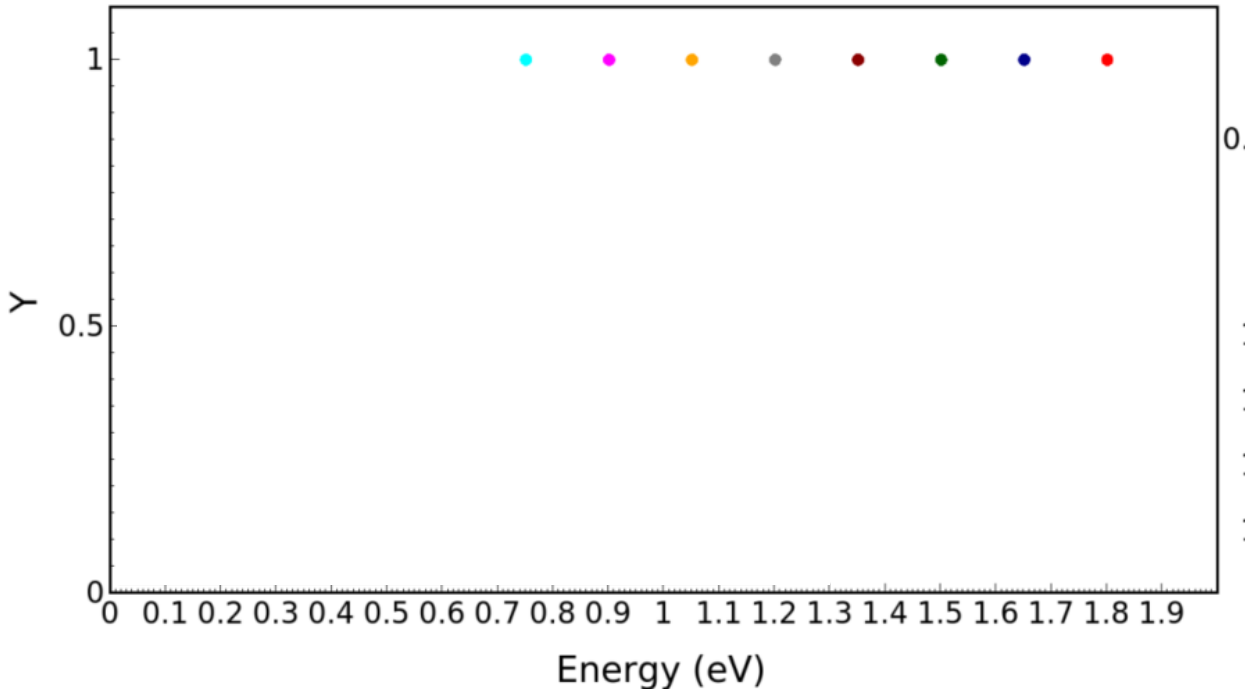


• a-Si:H.par: Effect of the Traps

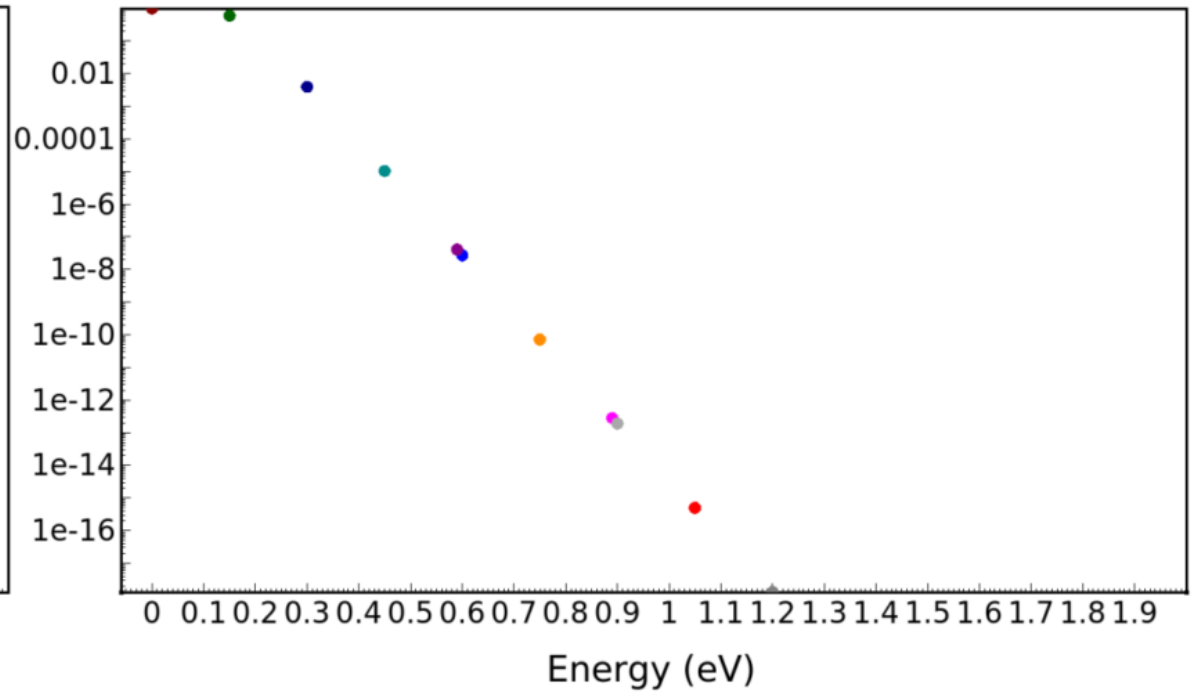
- Intrinsic a-SiH material
- Occupation probability of Traps is almost always 0

1st Study was to invert the traps type to investigate the effects on the device behavior

DONOR



ACCEPTOR



• a-Si:H.par: Effect of the Traps (3)