Self consistent solution of Schrodinger- Poisson equation

Course Supervisor

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Project group 3

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Research problem and achieved status

Research Problem:

Aiming to solve self-consistently the Schrodinger-Poisson equation for Uniform and Non-uniform meshing

Approach Adapted: Same as adapted in research paper

Achieved:

- Could self-consistently solved using Uniform meshing for Heterostructure
- Could manage to solve for Non-uniform meshing up to Carrier density distribution.

Presentation Flow

- **Introduction to self-consistent solver**
- **Discussing the uniform and Non-meshing Hamiltonian**
- **Simulation details and assumptions**
- **Results**

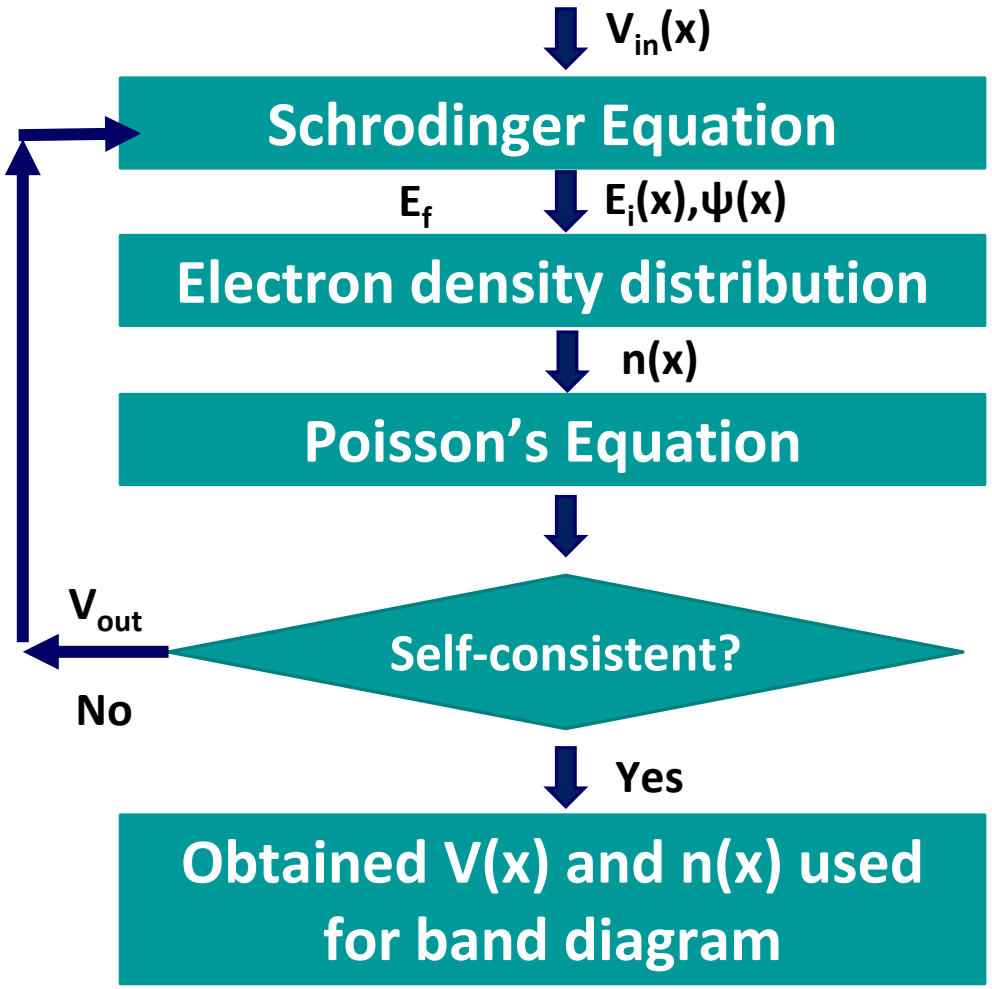
  1. Uniform meshing for Heterostructure QW (1)
     - Variations with band offset and doping
  2. Uniform meshing for Heterostructure QW(2)
     - Comparing results with online simulator and paper

- **Conclusion**

Self- Consistent Solver (SC solver)

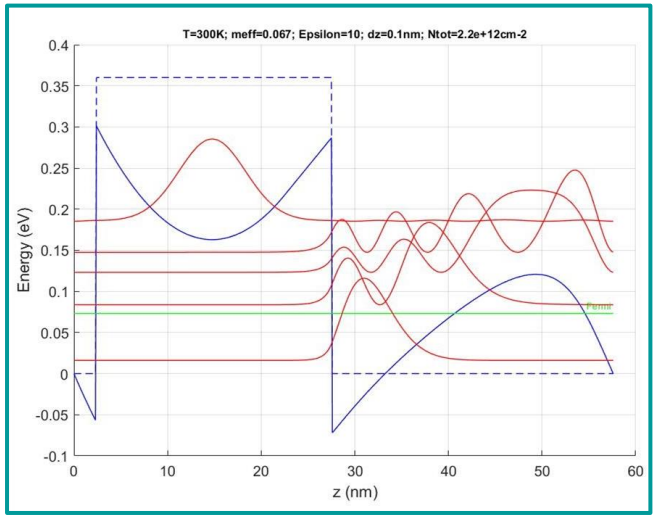
Gives the self-consistent solution for potential (V) profile and the charge density (n) profile

Basic flow chart for SC solver



$$-\frac{\hbar^2}{2}\frac{d}{dx}\left(\frac{1}{m^*(x)}\frac{d}{dx}\right)\psi(x)+V(x)\psi(x)=E\psi(x\Big)$$

$$n_k=\frac{m^*}{\pi\hbar^2}\int_{E_k}^{\infty}\frac{1}{1+e^{(E-E_F)/kT}}dE$$



$$n(x)=\sum_{k=1}^{m}\psi_k^*(x)\,\psi_k(x)n_k$$

$$\frac{d}{dx}\left(\varepsilon_s(x)\frac{d}{dx}\right)\phi(x)=\frac{-q[N_D(x)-n(x)]}{\varepsilon_0}$$

$$V(x)=-q\phi(x)+\Delta E_c(x)$$

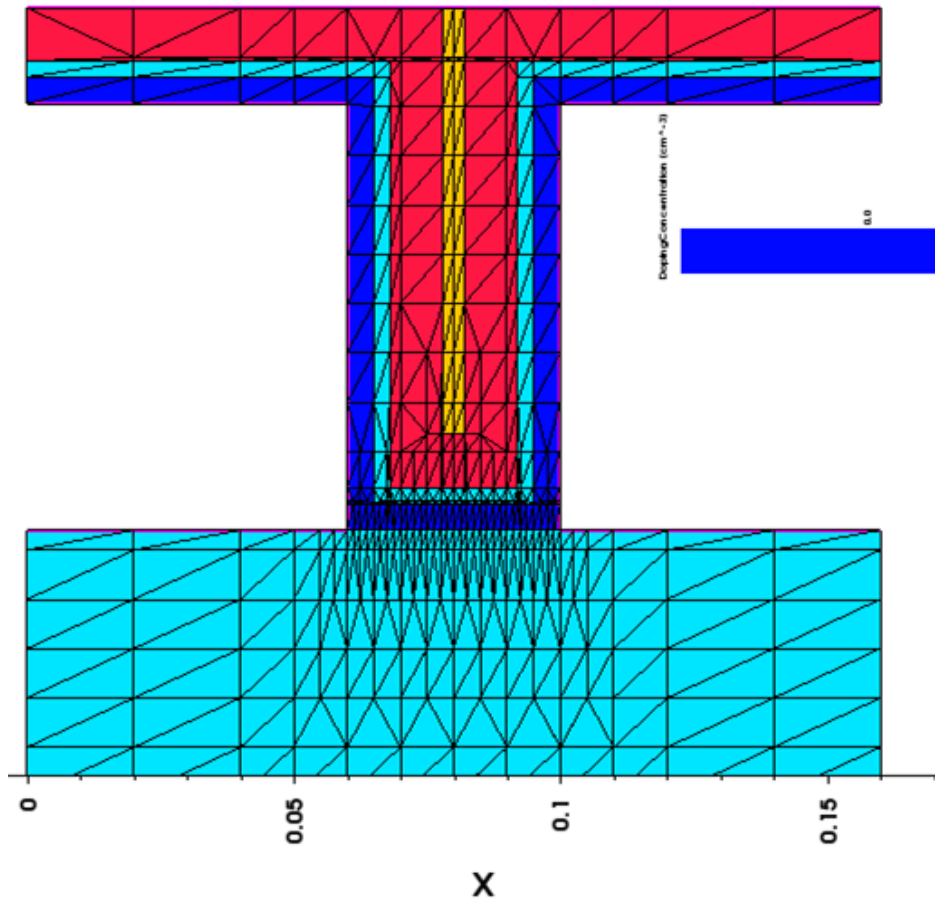
Uniform and Non-uniform mesh

The meshing type determines the symmetric nature of Hamiltonian

Need of non-uniform mesh

- The mesh is defined to solve equation at each node point to capture the physics
- The number of grid points more the computational load and time
- Trade off between the accuracy and computational resources/ time
- Different meshing scheme optimizes the solution and computational efficiency

The finer mesh is used where exact physic needs to be computed exactly, but finer mesh size causes issue of convergence.(At interface, channel)



Solving Schrodinger's equation

- In order to numerically solve the Schrodinger equation, we may discretize the differential equation (3) by using a three-point finite difference scheme

$$-\frac{\hbar^2}{2}\left(\frac{2(\psi_{i+1}-\psi_i)}{m_{i+1/2}h_i(h_i+h_{i-1})}-\frac{2(\psi_i-\psi_{i-1})}{m_{i-1/2}h_{i-1}(h_i+h_{i-1})}\right)=\lambda\psi_i.$$

This may be cast in the form of a matrix equation,

$$\sum_{j=1}^{n} A_{ij}\psi_j=\lambda\psi_i,$$

where

$$A_{ij}=\begin{cases}-\frac{\hbar^2}{2}\left(\frac{2}{m^*_{i+1/2}}\frac{1}{h_{i+1}(h_i+h_{i-1})}\right) & \text{if } j=i+1,\\ -\frac{\hbar^2}{2}\left(\frac{2}{m^*_{i-1/2}}\frac{1}{h_{i+1}(h_i+h_{i-1})}\right) & \text{if } j=i-1,\\ -A_{ii+1}-A_{ii-1}+V_i & \text{if } j=i,\\ 0 & \text{otherwise.}\end{cases} \quad (8)$$

For uniform meshing

$$L_i^2=(h_i+h_{i-1})/2,$$

Eq. (8) becomes

$$A_{ij}=\begin{cases}-\frac{\hbar^2}{2}\left(\frac{1}{m^*_{i+1/2}}\frac{1}{h_i}\right)\frac{1}{L_i^2} & \text{if } j=i+1,\\ -\frac{\hbar^2}{2}\left(\frac{1}{m^*_{i-1/2}}\frac{1}{h_{i-1}}\right)\frac{1}{L_i^2} & \text{if } j=i-1,\\ -A_{ii+1}-A_{ii-1}+V_i & \text{if } j=i,\\ 0 & \text{otherwise.}\end{cases}$$

We set $B_{ij}=L_i^2A_{ij}$, or in matrix notation,

$$B=MA,$$

For Non-uniform meshing

$$\sum_{j=1}^{n} A_{ij}\psi_j=\lambda\psi_i,$$

Making the Matrix Symmetric

- The matrix A which we constructed resembles the original Hamiltonian, however it is not symmetric anymore. The following method is presented in the paper to symmetrize the matrix which makes it easier to compute its eigenvalues and eigenvectors. Note that A is tridiagonal and L is symmetric (its diagonal elements are

$$B\psi = MA\psi = \lambda M\psi$$

$$M = LL$$
$$L^{-1}BL^{-1}\psi = L^{-1}LA\psi = \lambda L^{-1}LL\psi$$

$$L_i^2 = (h_i + h_{i-1})/2$$

$$H\Phi = \lambda\Phi$$
$$where$$
$$H = L^{-1}BL^{-1} \,\&\, \psi = L^{-1}\Phi$$

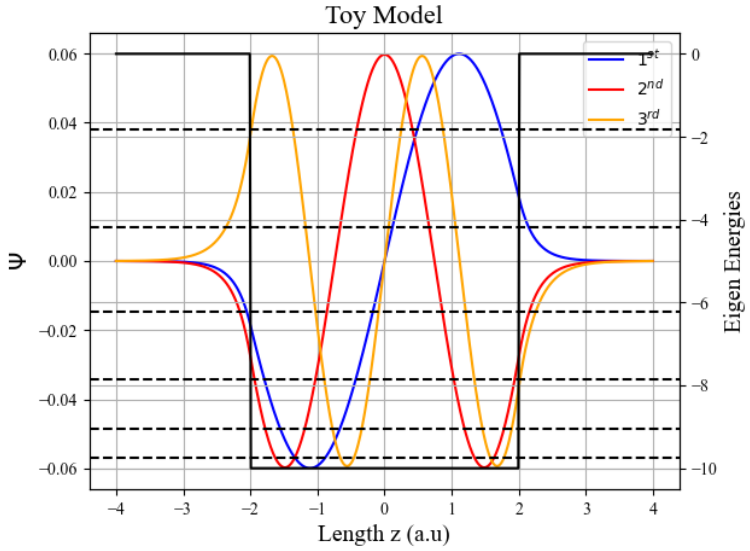
- Here, B is tridiagonal (as M is diagonal and A is tridiagonal). H is the symmetric matrix whose eigenvalues are same as that of A, and eigenvectors are related to the eigenvectors of A by the last relation. We implemented this in Python and obtained the results for eigenstates of a Quantum Well

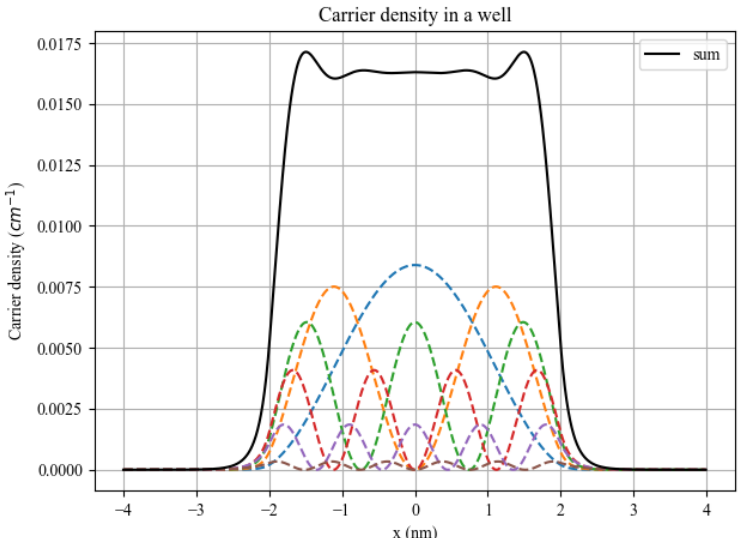
Simulations to Validate Effectiveness of Non Uniform Mesh

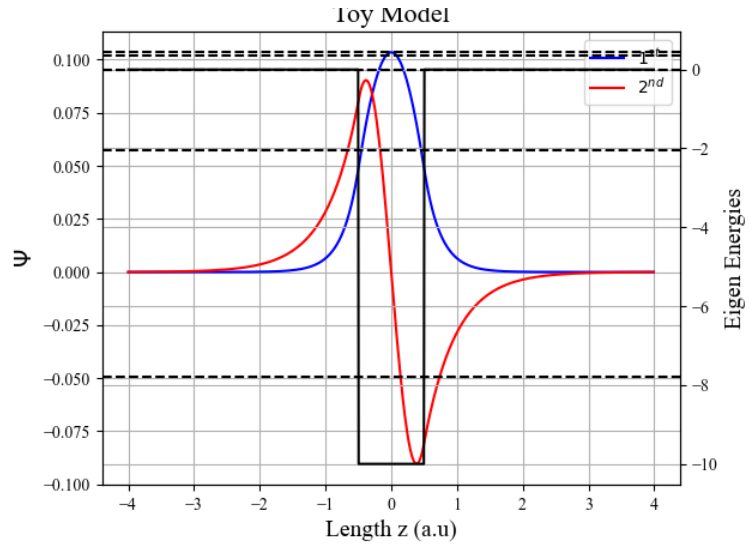
No. of Points	Type of Mesh	Details of NonUniform Mesh	Energy level difference	Time Taken	Accuracy
5000	Uniform		0.2498820096	170.5040636	Reference
2000	Uniform	-	0.249725558	13.89884853	99.93738979
2000	Non Uniform	250-1500-250	0.2496642333	17.41671896	99.91284835
2000	Non Uniform	100-1800-100	0.2497168643	19.47167683	99.93391069
1500	Uniform	-	0.2508900603	6.531668186	99.59658932
1500	Non Uniform	250-1000-250	0.2495059325	7.636870384	99.84949813
1500	Non Uniform	50-1400-50	0.2503135147	7.655210257	99.82731645
1500	Non Uniform	100-1300-100	0.2496155905	7.115903378	99.89338204
1000	Uniform	-	1.39883184	3.877412558	Erreneous
1000	Non Uniform	50-900-50	0.2494530296	2.65678525	99.82832699
500	Uniform	-	2.407057438	0.74503088	Erreneous
500	Non Uniform	10-480-10	0.2489872221	0.6521549225	99.64191599

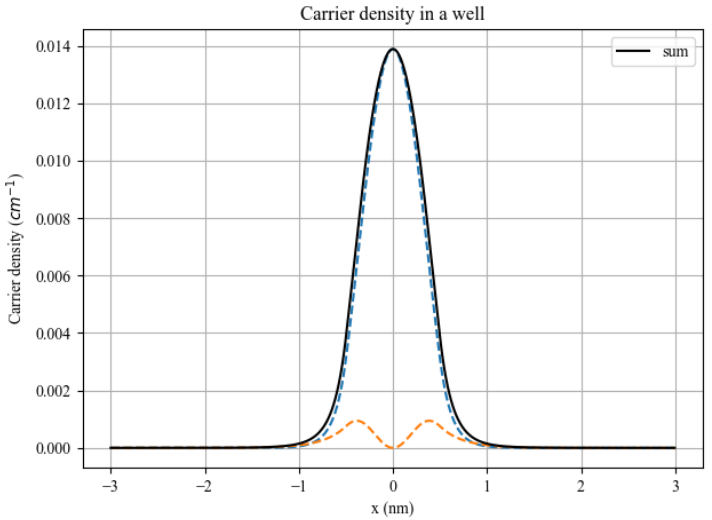
Non uniform mesh clearly offers a better Accuracy/Computational time ratio. Also, as we are using less number of points, data storage requirements are also relaxed and we get results with good accuracy.

profile


Toy Model
1st
2nd
3rd
Ψ
Eigen Energies
Length z (a.u)


Carrier density in a well
sum
Carrier density (cm^{-1})
x (nm)


Toy Model
1st
2nd
Ψ
Eigen Energies
Length z (a.u)


Carrier density in a well
sum
Carrier density (cm^{-1})
x (nm)

Simulation Details

The assumptions and the parameter/tool used

Simulation Details

- Self-consistently solving Schrodinger- Poisson's equation for calculating electron density distribution, electric-field and potential profile.

  two structures

  1. Toy model with uniform meshing
  2. 1D Heterostructure with uniform meshing
  3. Toy model with non-uniform meshing

  (Variation parameters: Doping, off-set, Mesh size)

Coding Languages: Python/ MATLAB

Tools: 1-D heterostructure simulator NanoHUB

Tool on the nanoHUB: 1D Heterostructure .http://www.nanohub.org/tools/1dhetero

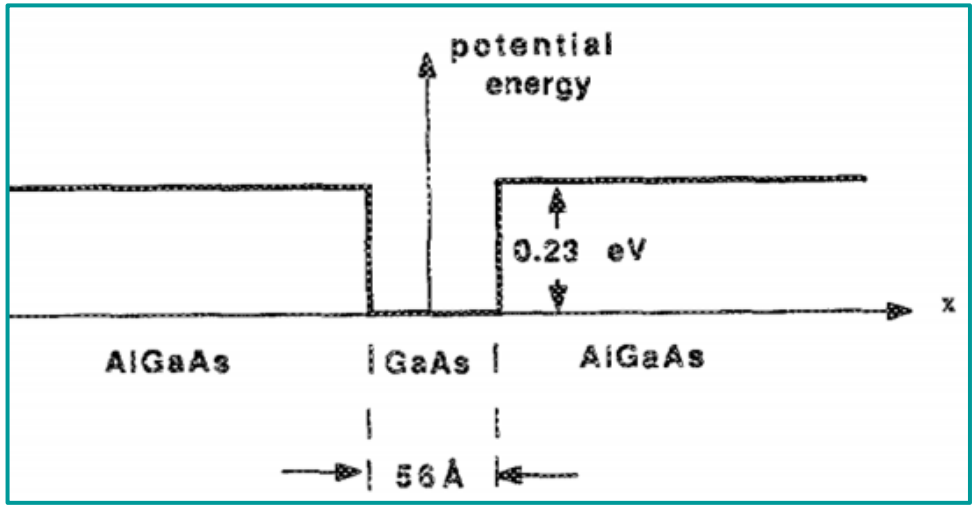
Constants and values taken

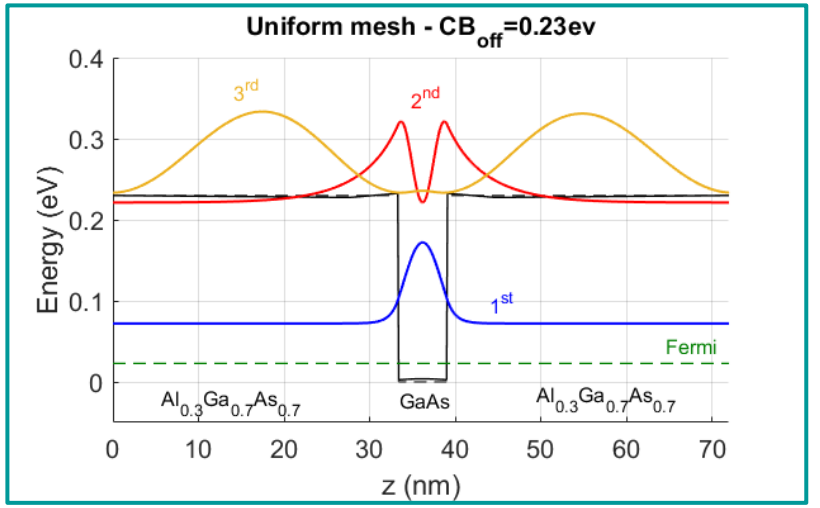
Material properties	GaAs (eV)	AlGaAs (eV)
Band gap(eV)	1.43	(varies 1.43 to 2.16)
Band Offset (eV)	Reference(0)	0.23 and 0.46
Dielectric constant(ε)	10	10
Effective mass	0.067 m_0	0.067 m_0

Assumptions for Simplicity:

- The dielectric constant value taken as constant (10) for all materials
- The effective mass of the material has also been taken constant (0.067 m_0)

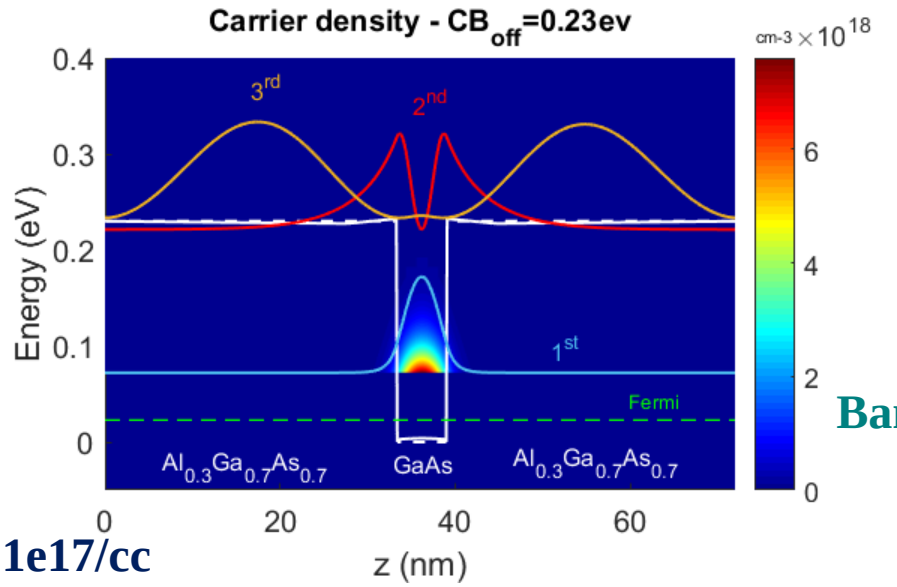
AlGaAs-GaAs QW(1)



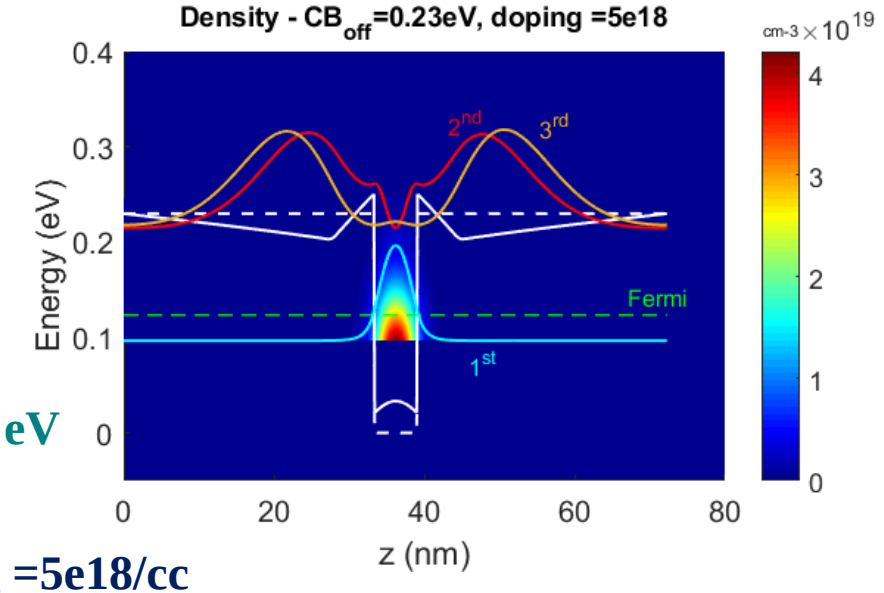


UNIFORM MESHING

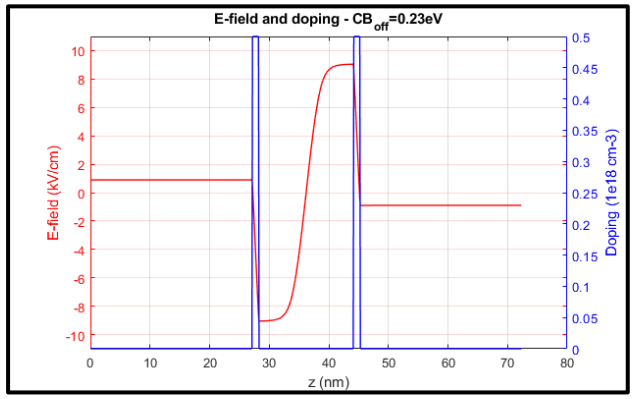
variation



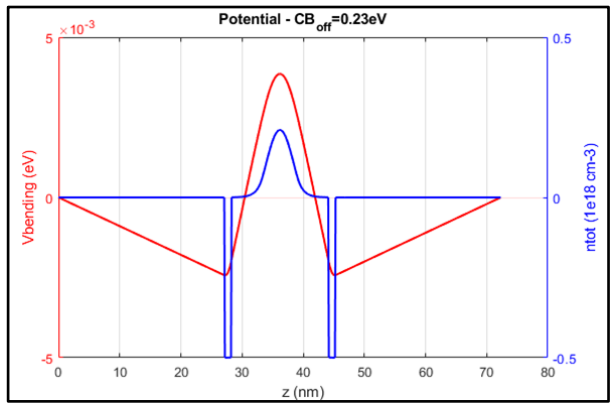
Band off-set=0.23 eV



Doping =1e17/cc

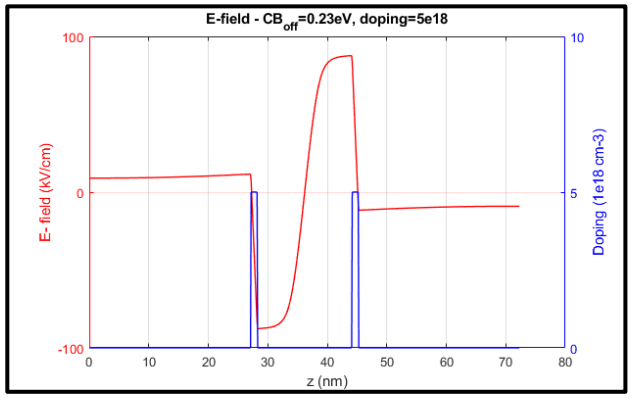


Electric and doping profile

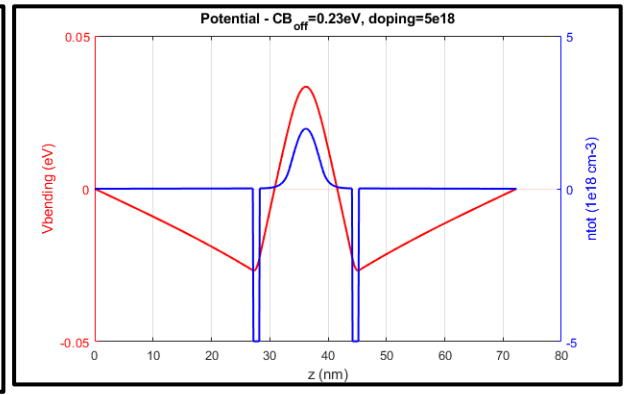


Potential and charge density

Doping =5e18/cc

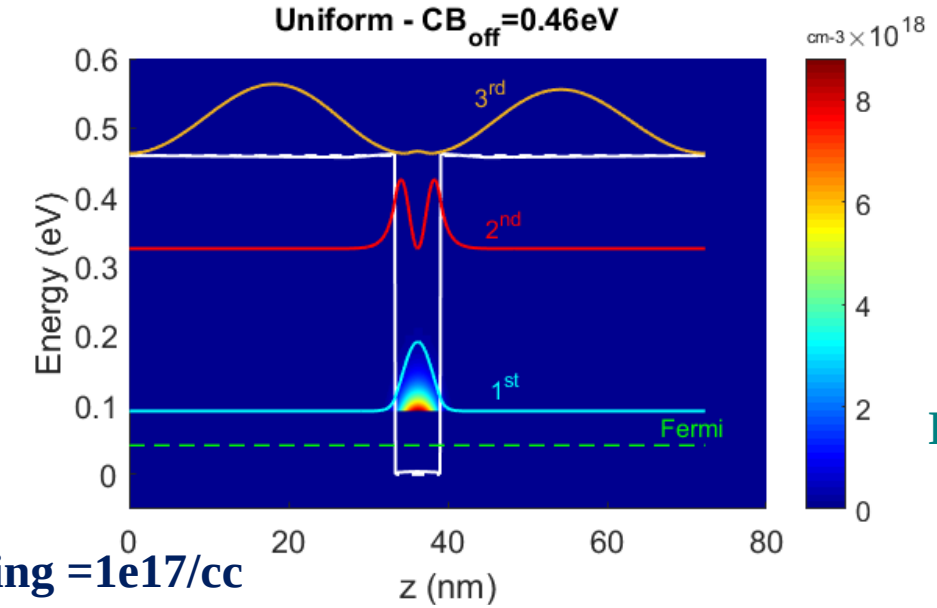


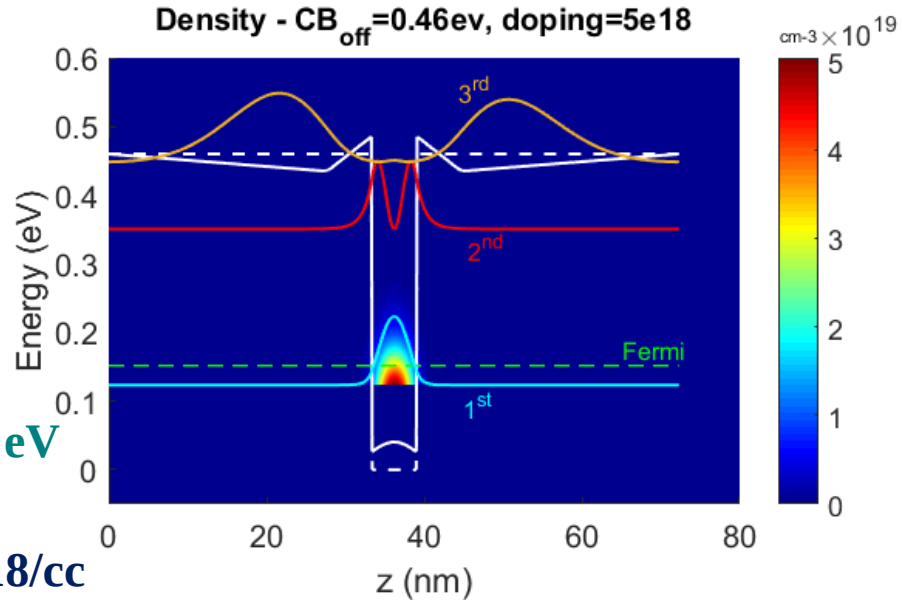
Electric and doping profile



Potential and charge density

variation

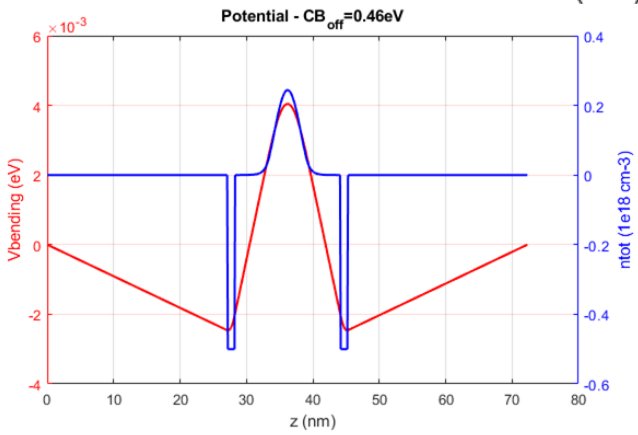




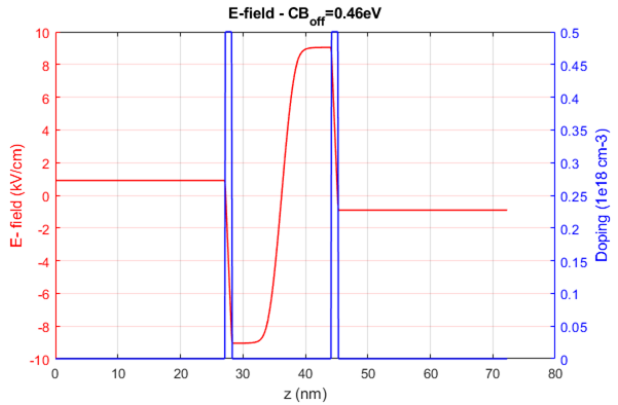
Band off-set=0.46 eV

Doping =1e17/cc

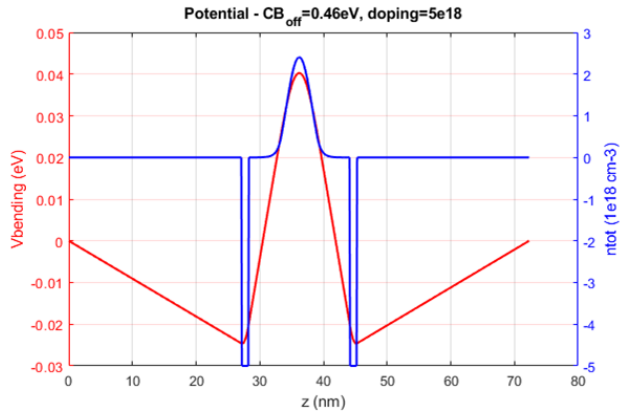
Doping =5e18/cc



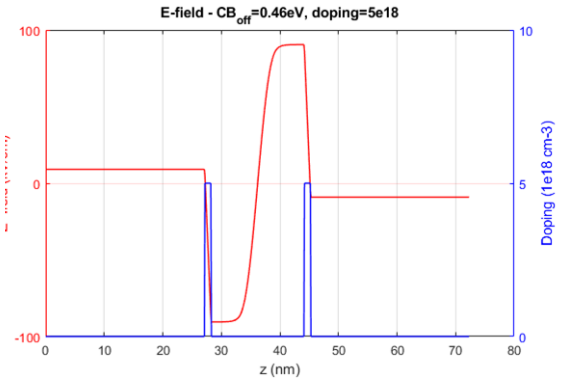
Electric and doping profile



Potential and charge density

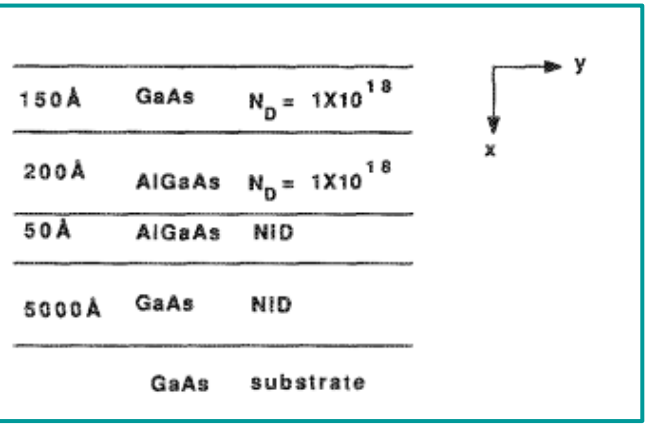


Electric and doping profile



Potential and charge density

Comparison Between Theory/Simulator/ and Code Structure



Paper

Heterostructure Review

Layer	Material System	n-Doping (cm-3)	Thick. (nm)	Mono- layers
Substr.	GaAs	1.e+14	1000.06	3538
L01	GaAs	1.e+14	500	1768
L02	AlGaAs	1.e+14	5	18
L03	AlGaAs	1.e+18	20	70
L04	GaAs	1.e+18	15.00	54

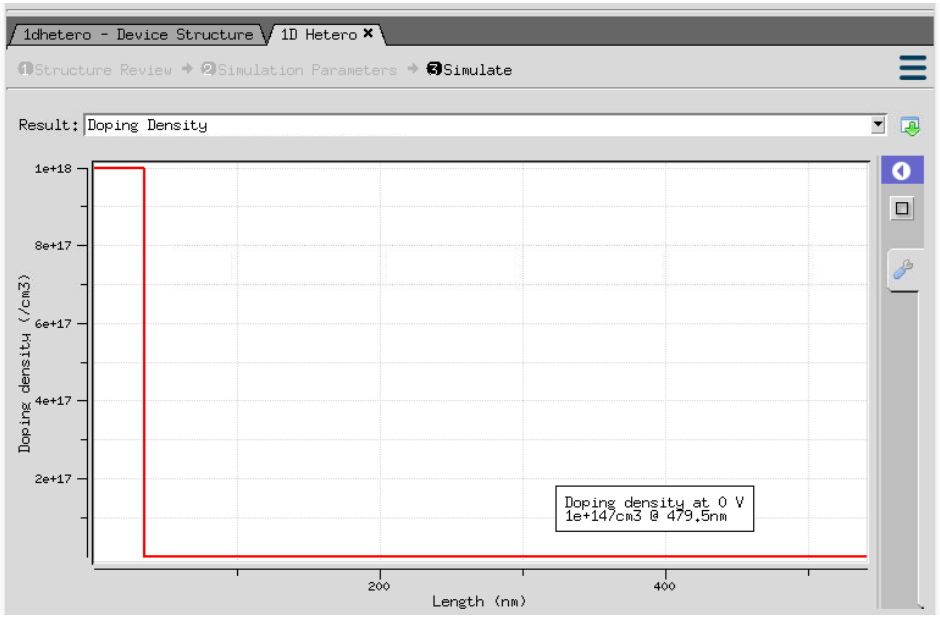
Online Simulator

Different Layers	Thickness in nm	Doping (*1e+18cc)
GaAS	2	1
AlGaAs	20	1
AlGaAs	5	0
GaAS	30	0

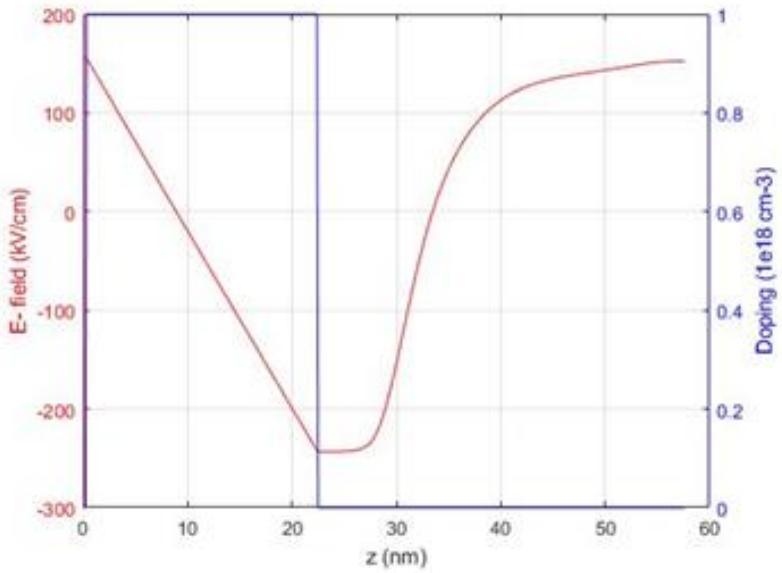
In Code

Simulated Biasing Condition

Doping Profile and Electric Field

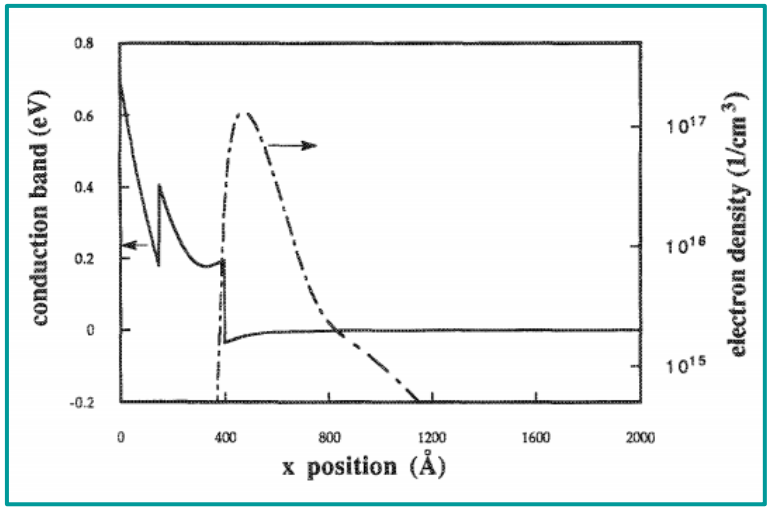


In Simulator

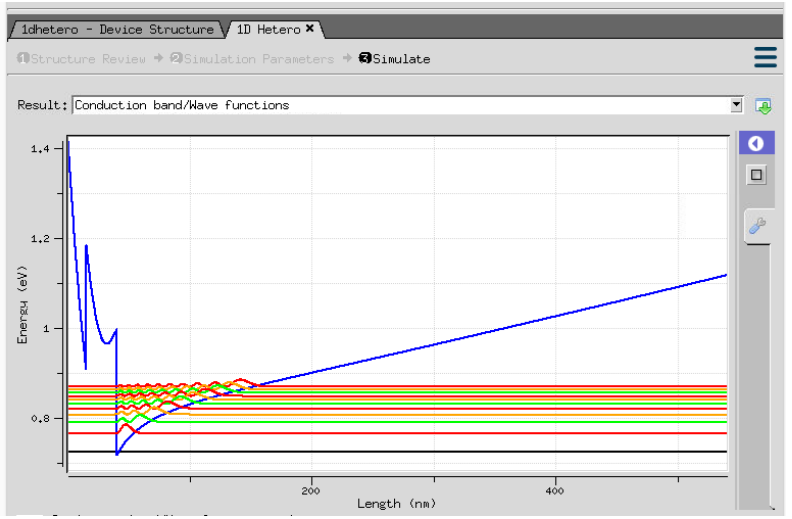


In Code

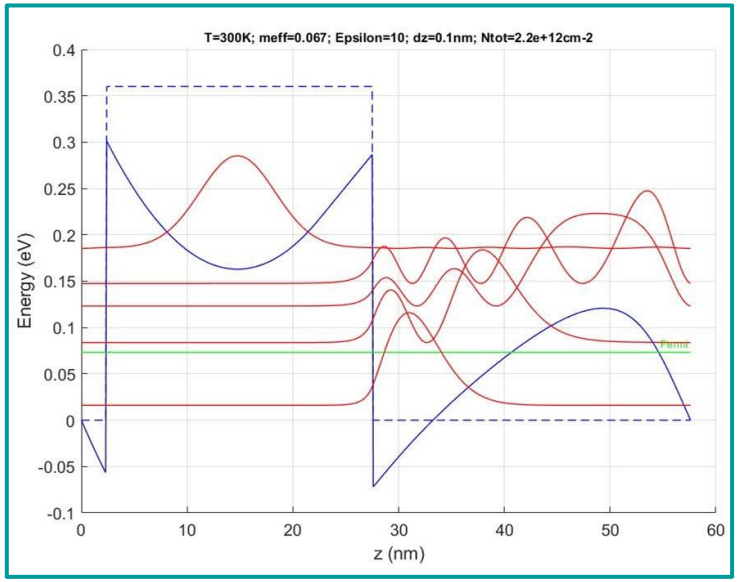
Conduction Band and wave Function



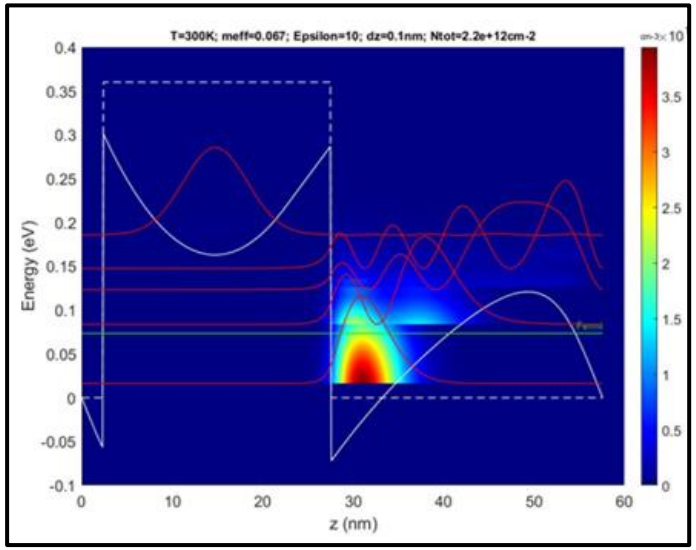
Paper



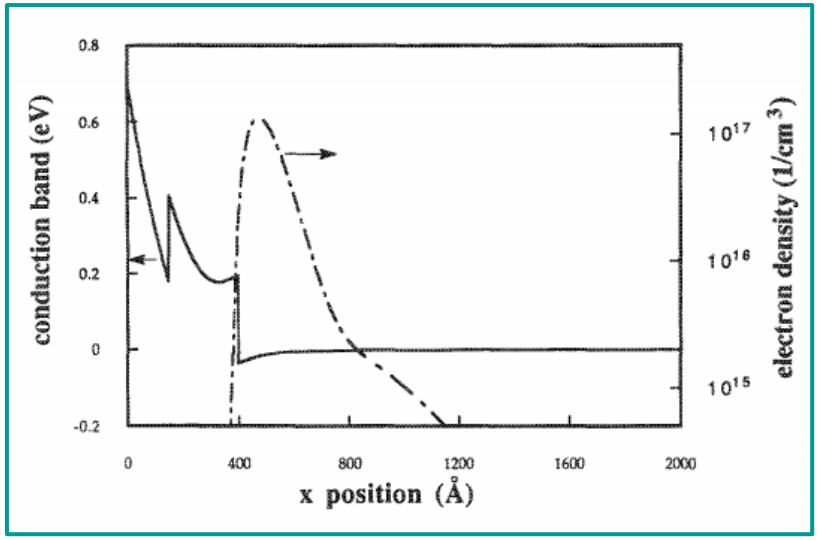
Online Simulator



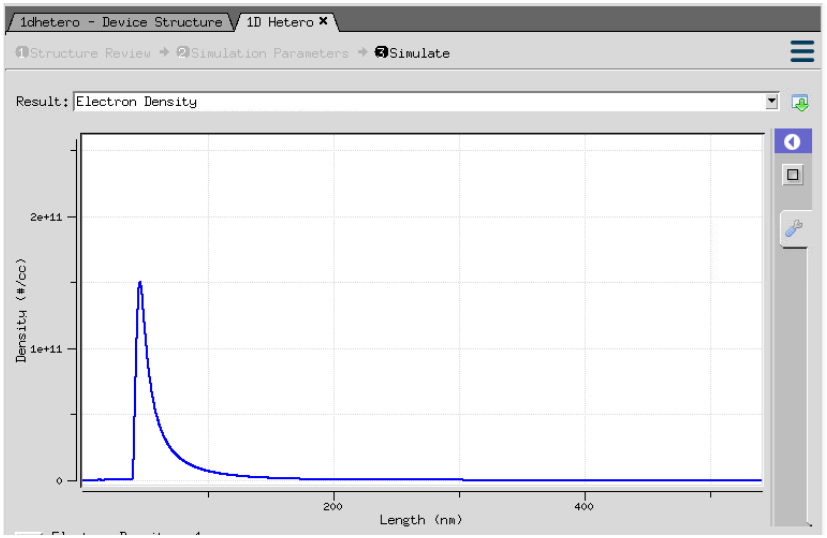
In Code



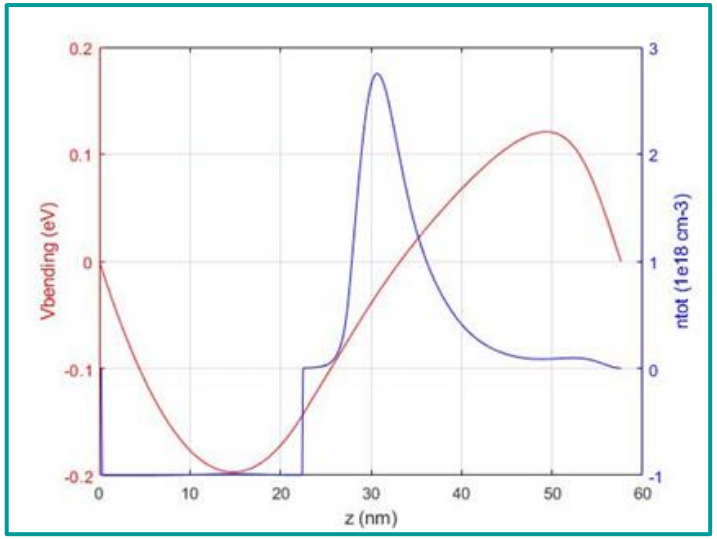
Carrier Density



Paper



Online Simulator

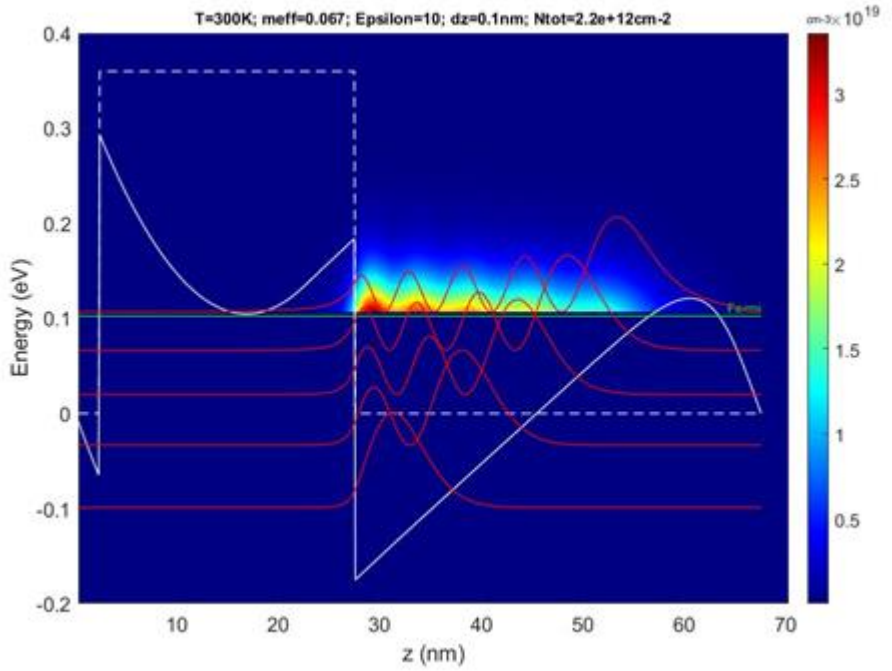


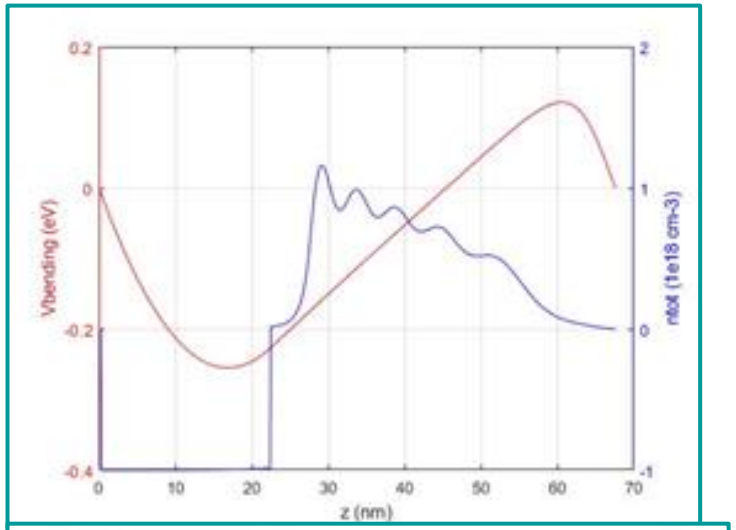
In Code

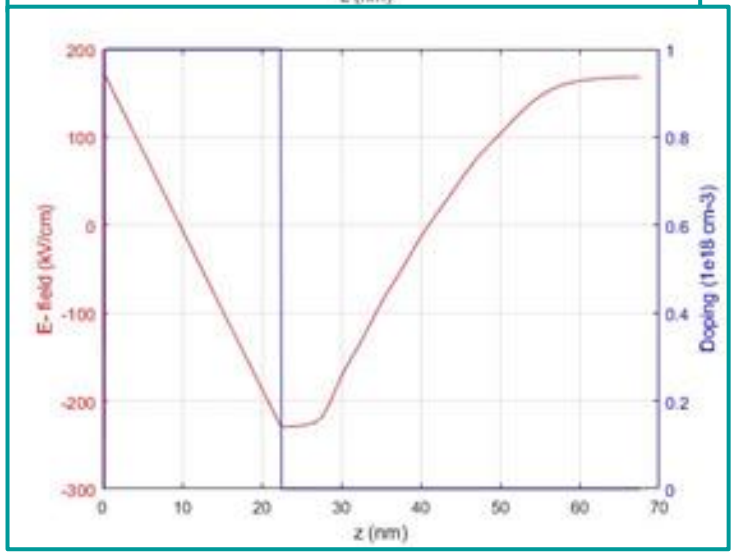
With Substrate thickness Variation

GaAs	0	0
GaAs	0	0
GaAs	2	1
AlGaAs40	20	1
AlGaAs40	5	0
GaAs	40	0

Thickness sub = 40 nm



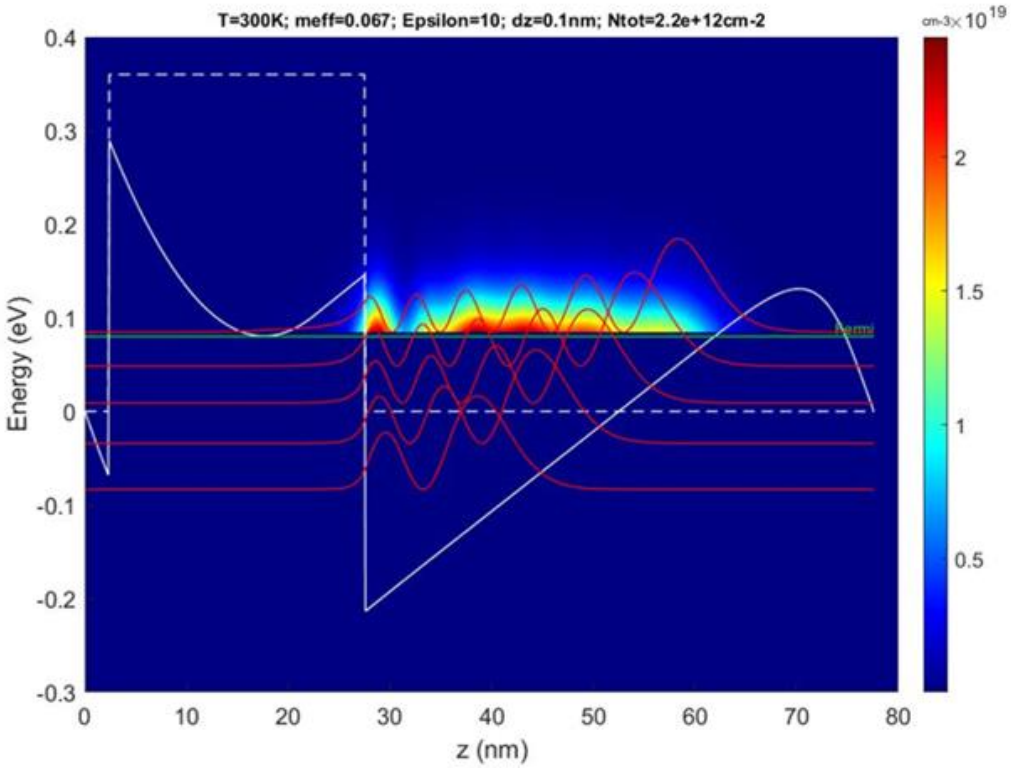


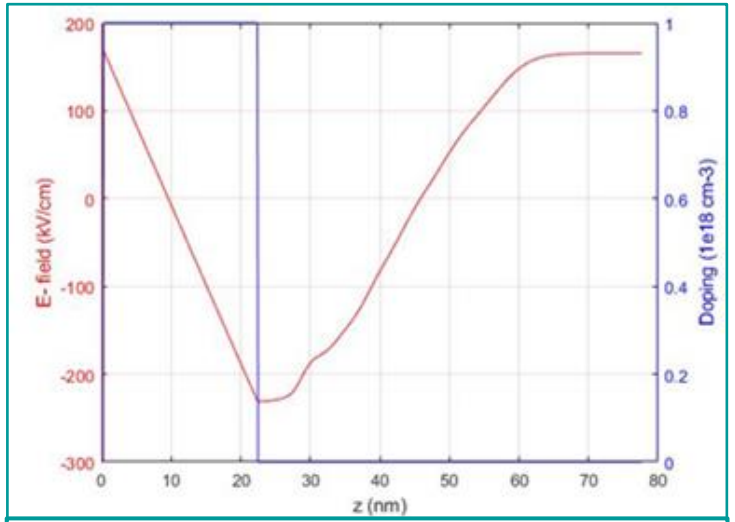


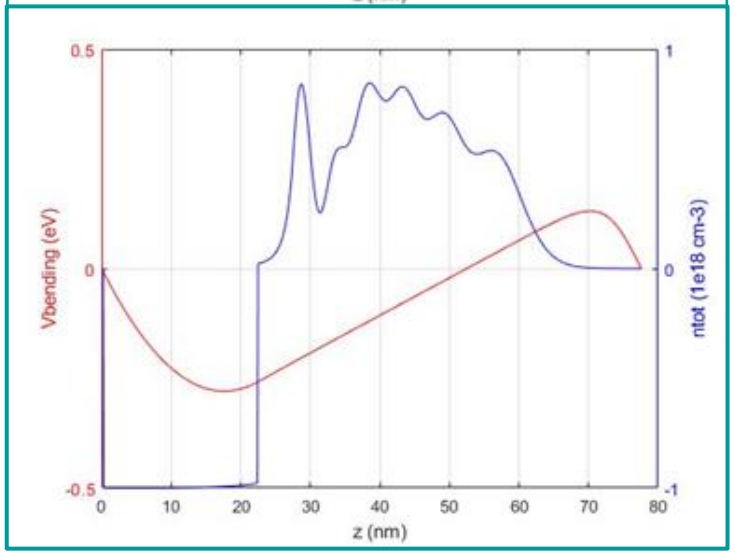
With Substrate thickness Variation

GaAs	0	0
GaAs	0	0
GaAs	2	1
AlGaAs40	20	1
AlGaAs40	5	0
GaAs	50	0

Thickness sub = 50 nm







With increasing substrate thickness number of bound states are increasing and carrier distribution approaching rectangular profile. with higher thickness the density profile move away from interface.

Conclusion

- Uniform meshing gives symmetric and Non-uniform gives asymmetric Hamiltonian

For Uniform meshing

- There is trade off between accuracy and computational resource utilization
- Bound states have proportional relation with band off-set and the thickness of barrier layer
- Carrier density also varies proportionately with doping.

Limitation:

Convergence issue for low doping and non- uniform meshing to solve self-consistently

References

- *Tan, I-H., G. L. Snider, L. D. Chang, and E. L. Hu. "A self-consistent solution of Schrödinger–Poisson equations using a nonuniform mesh." Journal of applied physics 68, no. 8 (1990): 4071-4076.*

- *Tan, I-H., G. L. Snider, L. D. Chang, and E. L. Hu. "A self-consistent solution of Schrödinger–Poisson equations using a nonuniform mesh." Journal of applied physics 68, no. 8 (1990): 4071-4076.*

Tools: 1-D heterostructure simulator NanoHUB

Tool on the nanoHUB: 1D Heterostructure .http://www.nanohub.org/tools/1dhetero

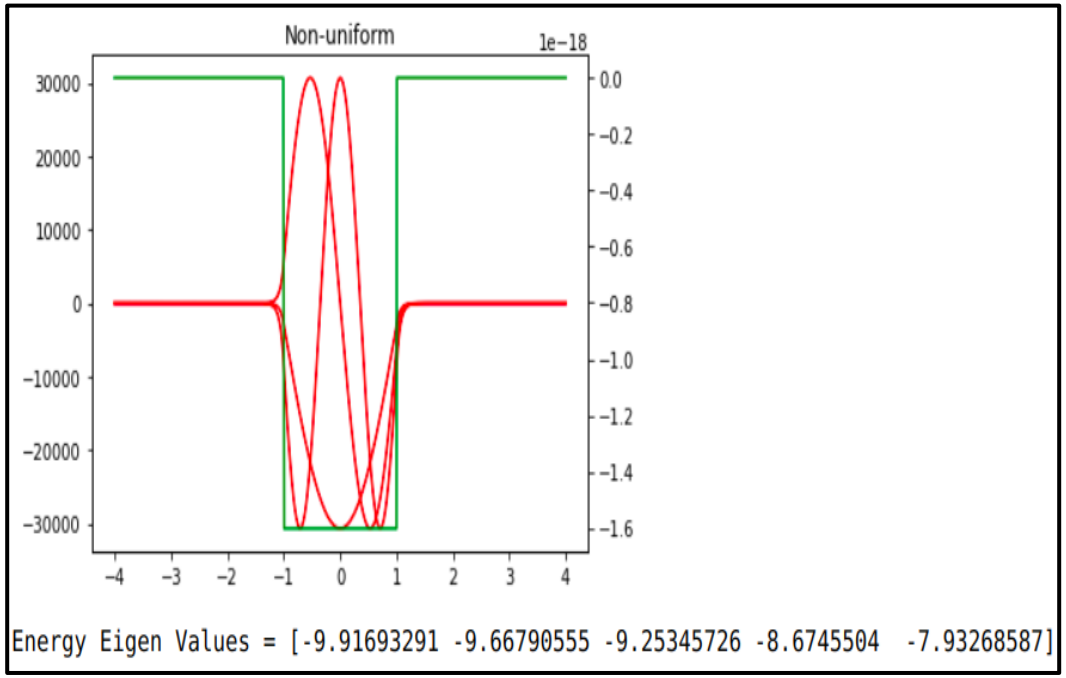
THANKS

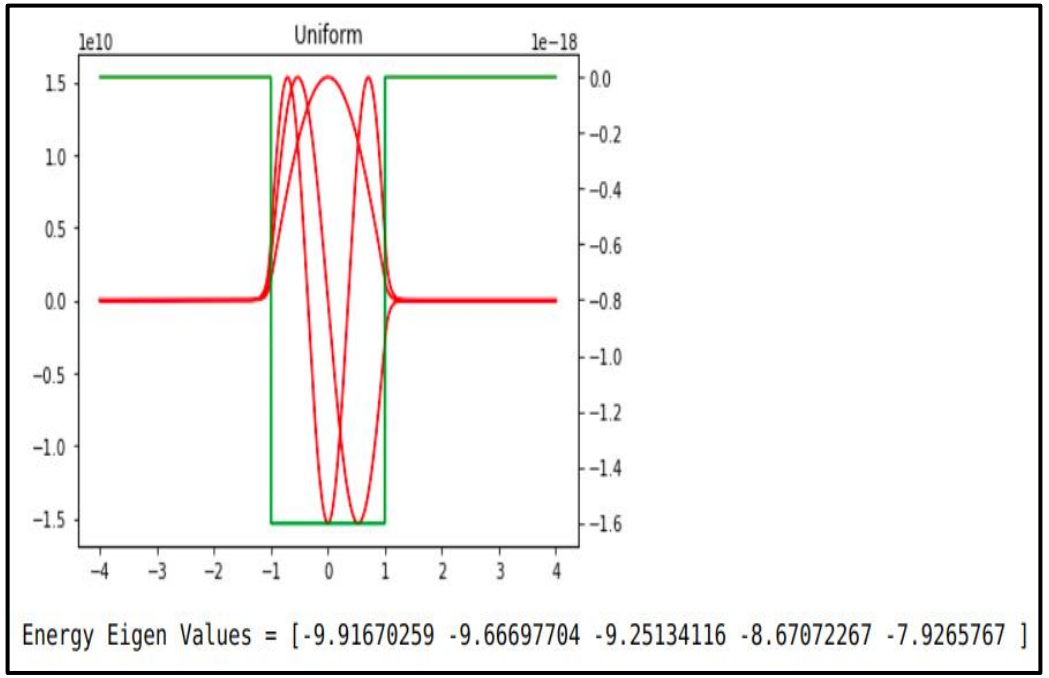
&

QUESTIONS

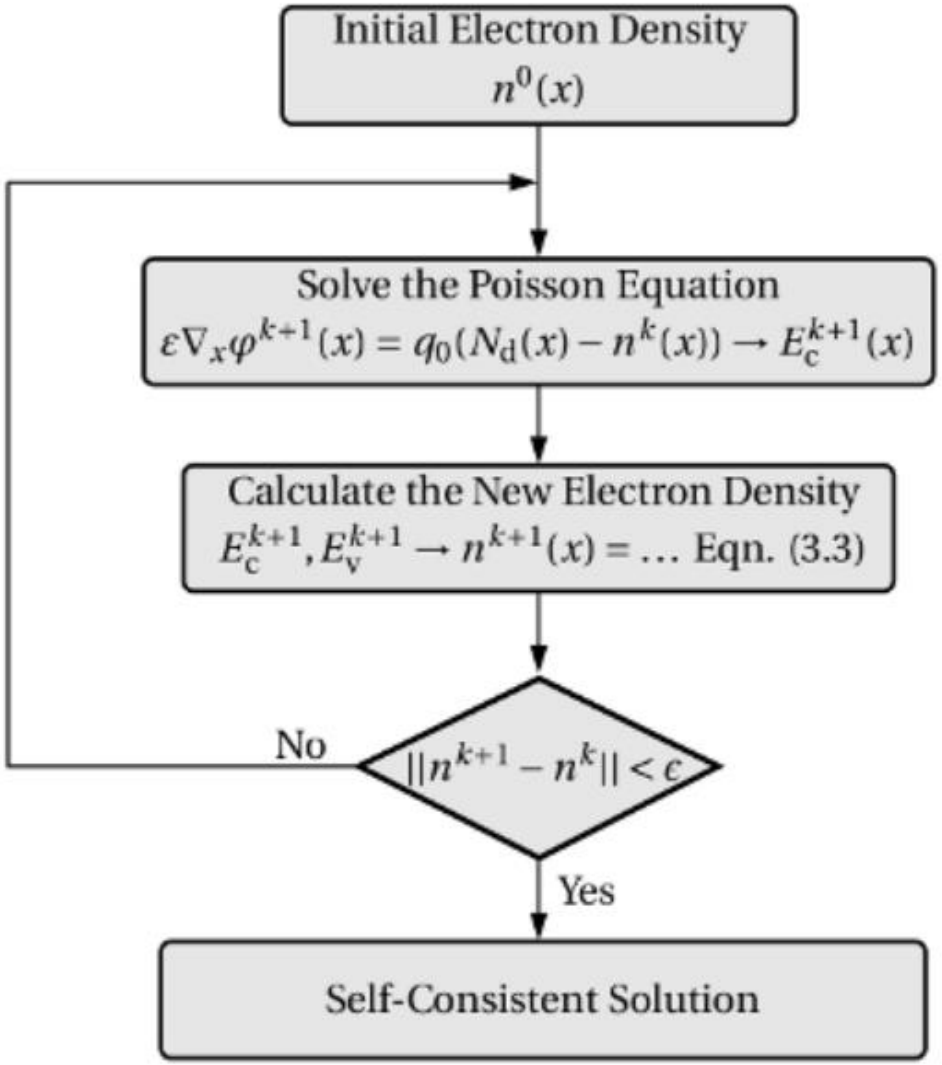
Preliminary Results of Non-uniform Mesh

- We get the same eigen energies and eigenvalues for a quantum well of depth 10V. Even though we used significantly lesser number of points for non-uniform mesh (1000 in total), we obtained the result in about 2.76s, whereas in case of uniform meshing, we required 2000 points for the accuracy which required about 12.5s for computation. We obtain the same eigen energies as shown below -

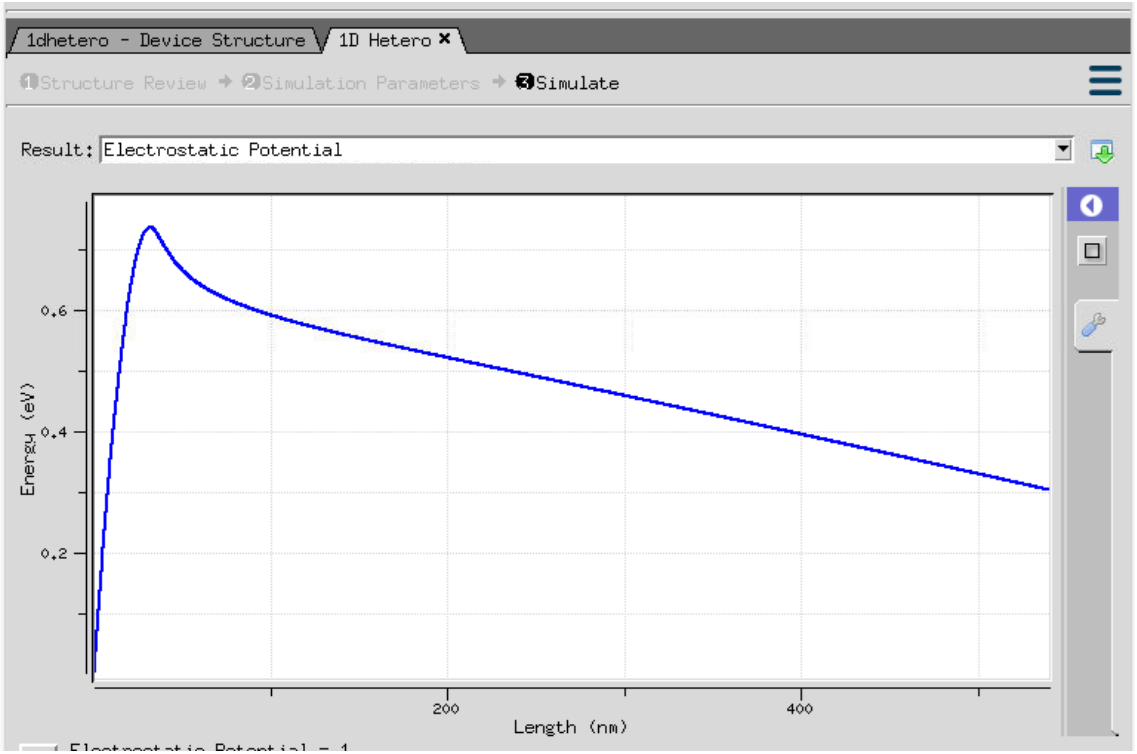




Poisson Solver



Electrostatic Potential



Simulator