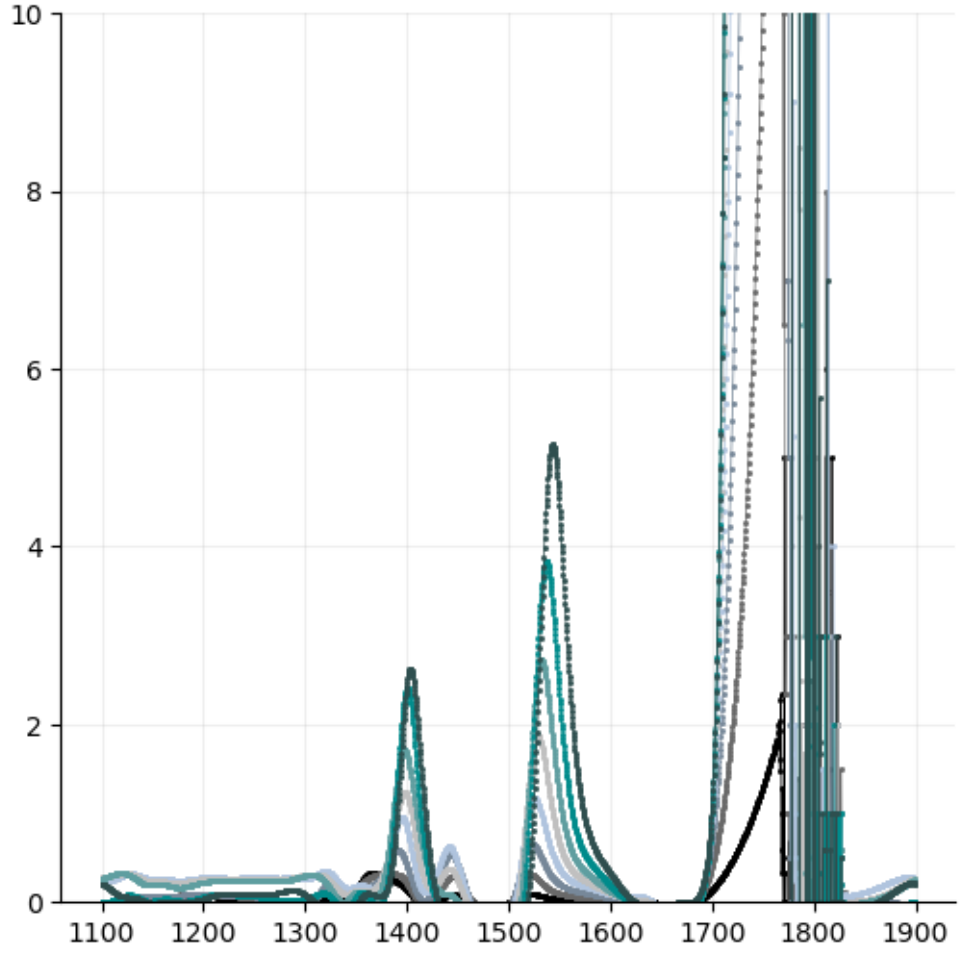
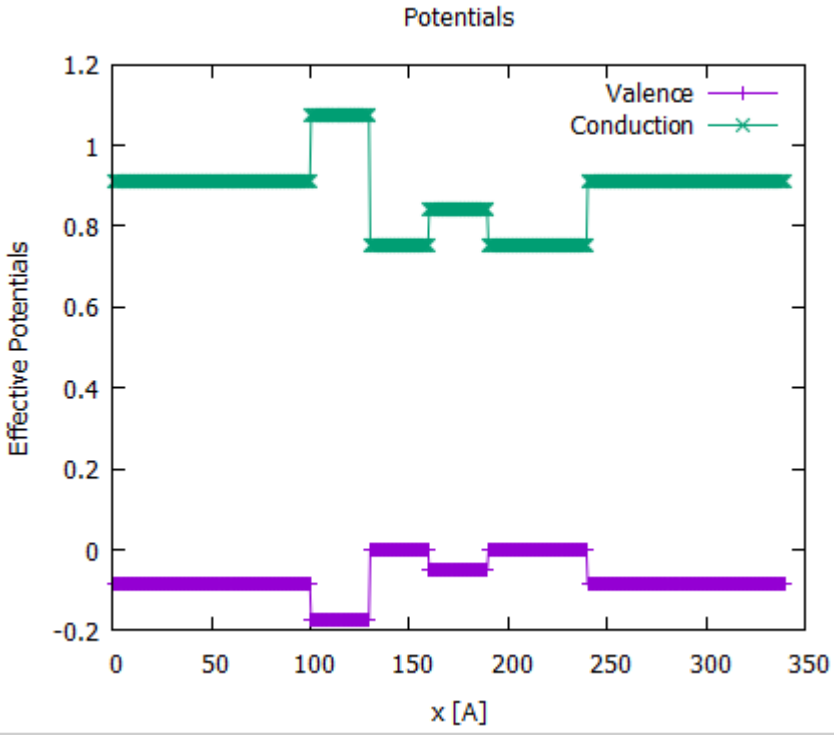
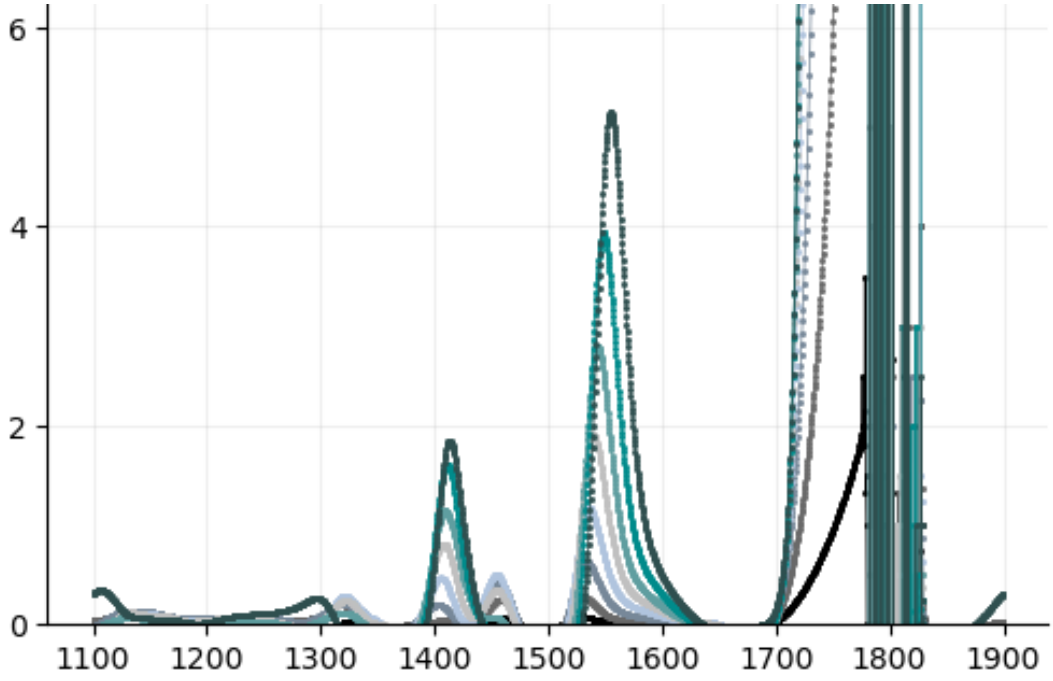
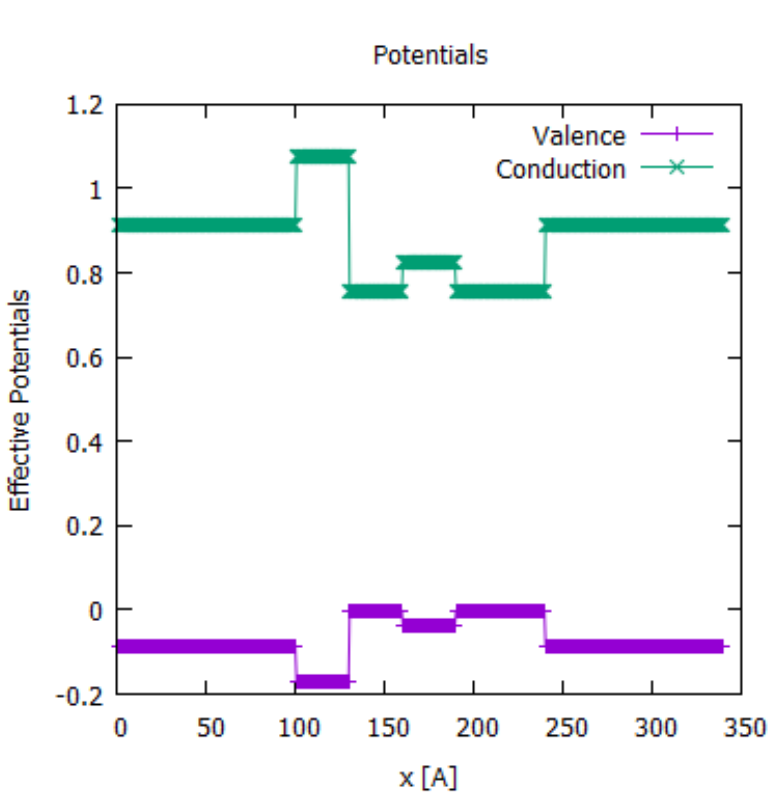
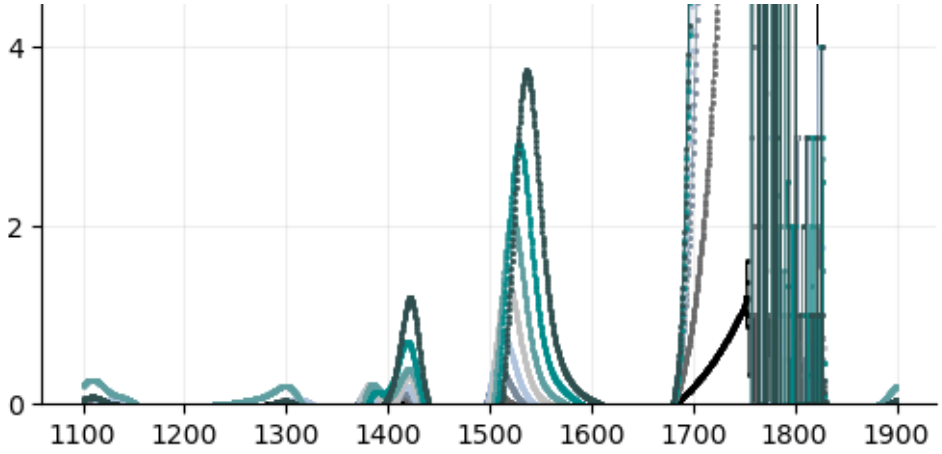
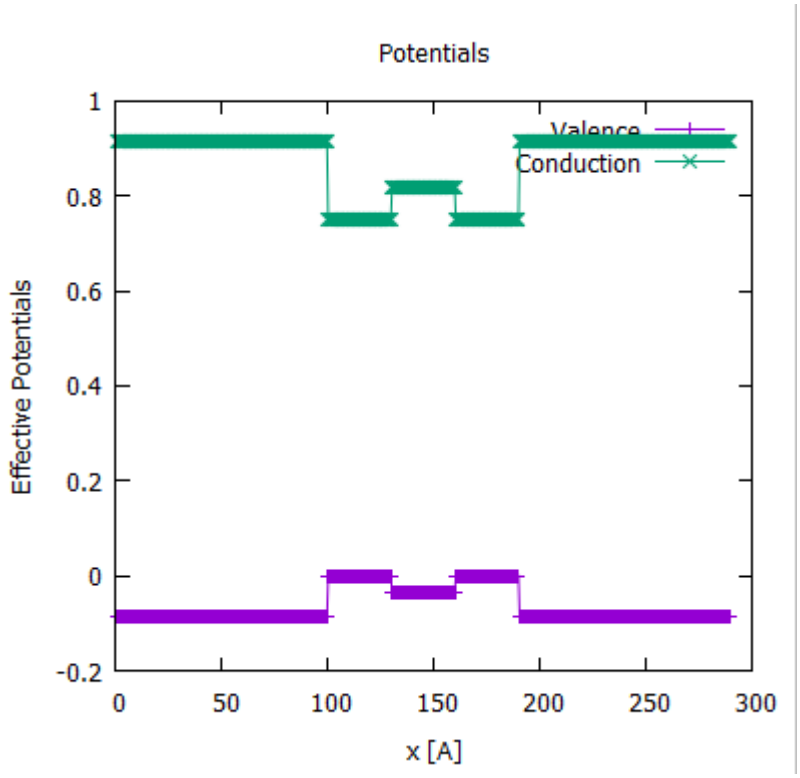

10
8
6
4
2
0
1100
1200
1300
1400
1500
1600
1700
1800
1900

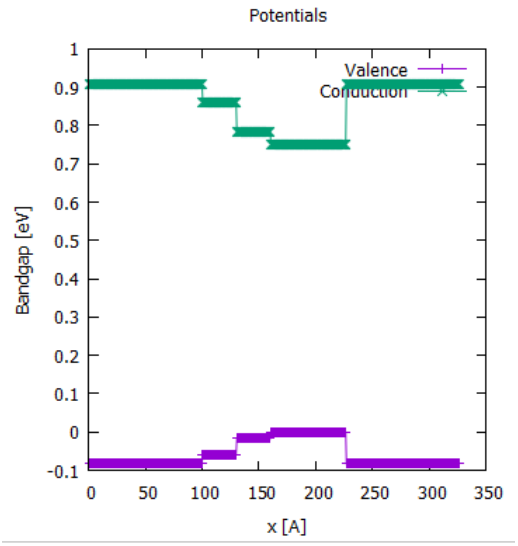

Potentials
Valence
Conduction
Effective Potentials
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
0
50
100
150
200
250
300
350
x [A]

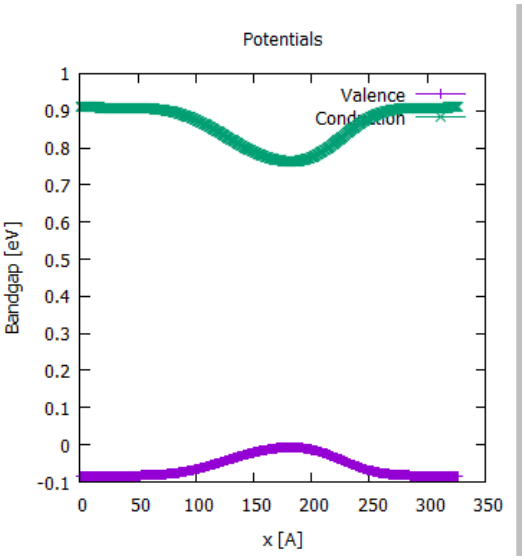

6
4
2
0
1100
1200
1300
1400
1500
1600
1700
1800
1900

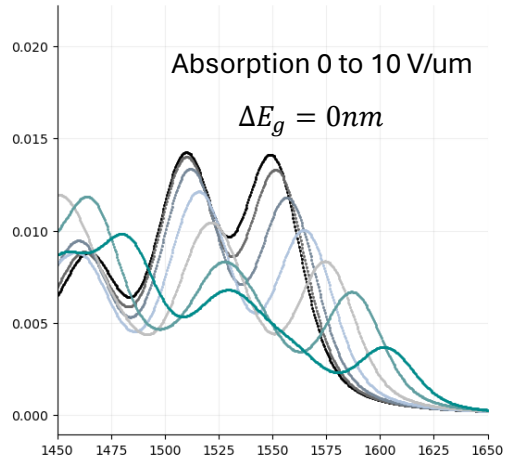

Potentials
Valence
Conduction
Effective Potentials
x [A]
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
0
50
100
150
200
250
300
350

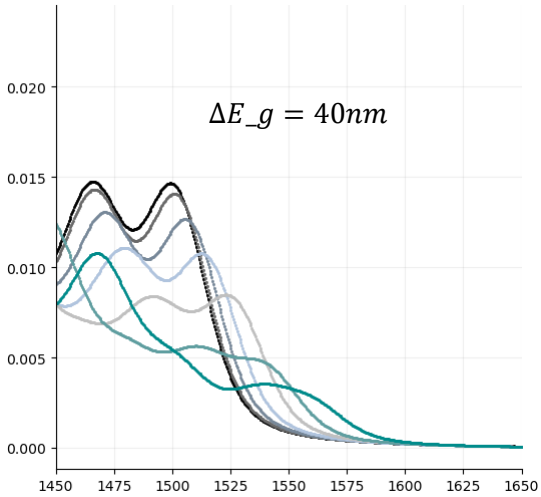

4
2
0
1100
1200
1300
1400
1500
1600
1700
1800
1900


Potentials
Valence
Conduction
Effective Potentials
1
0.8
0.6
0.4
0.2
0
-0.2
0
50
100
150
200
250
300
x [A]

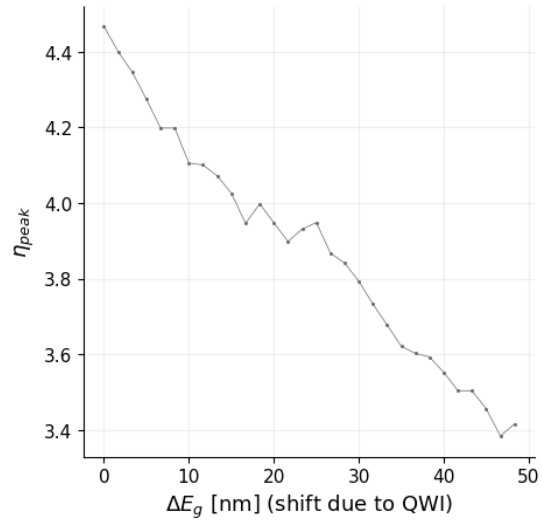


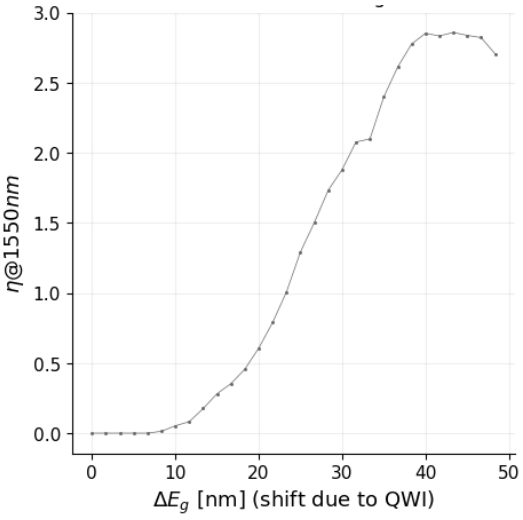






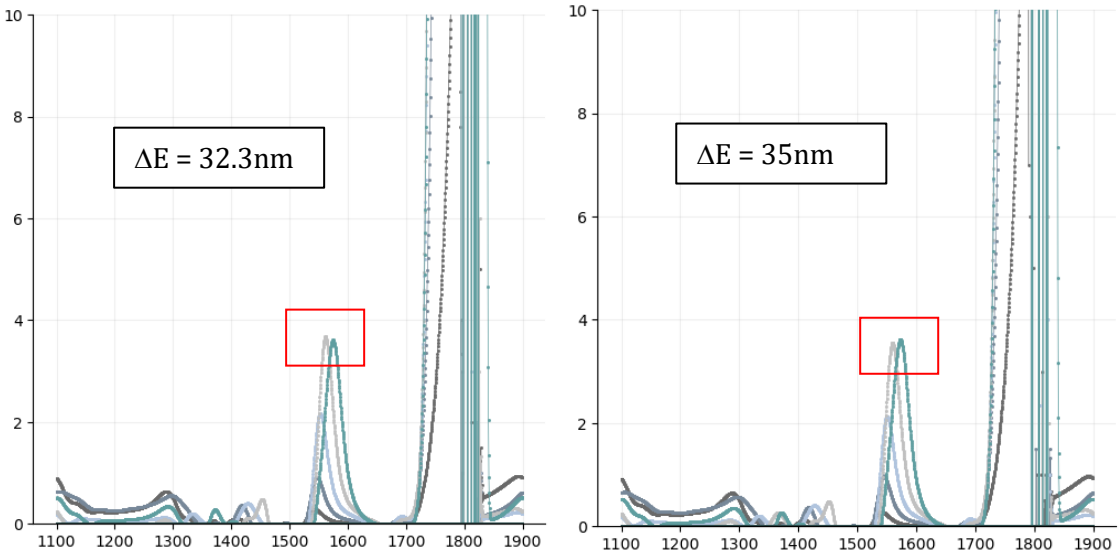
FOM evolution:

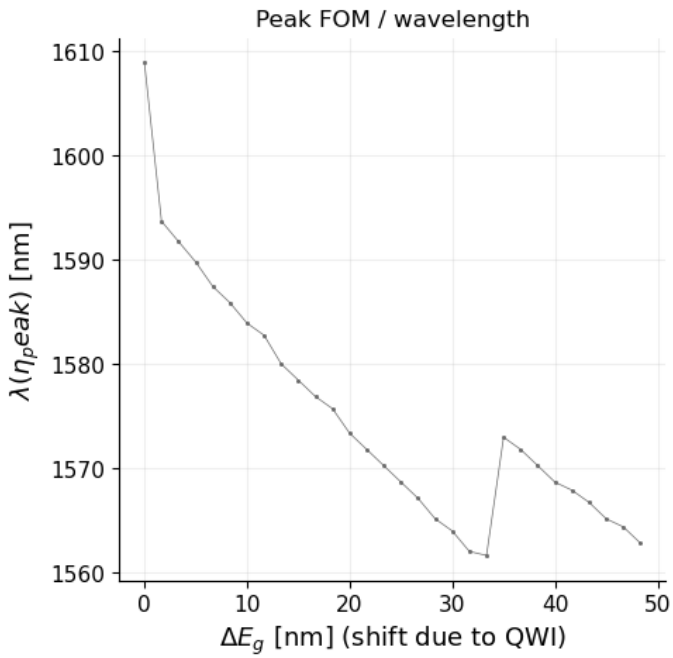




Odd effect:

FOM





This jump happened because I was simulating only 5 or 6 electric fields.

InP_layer2 = Layer(InGaAlAs_material(1039.85), 100)

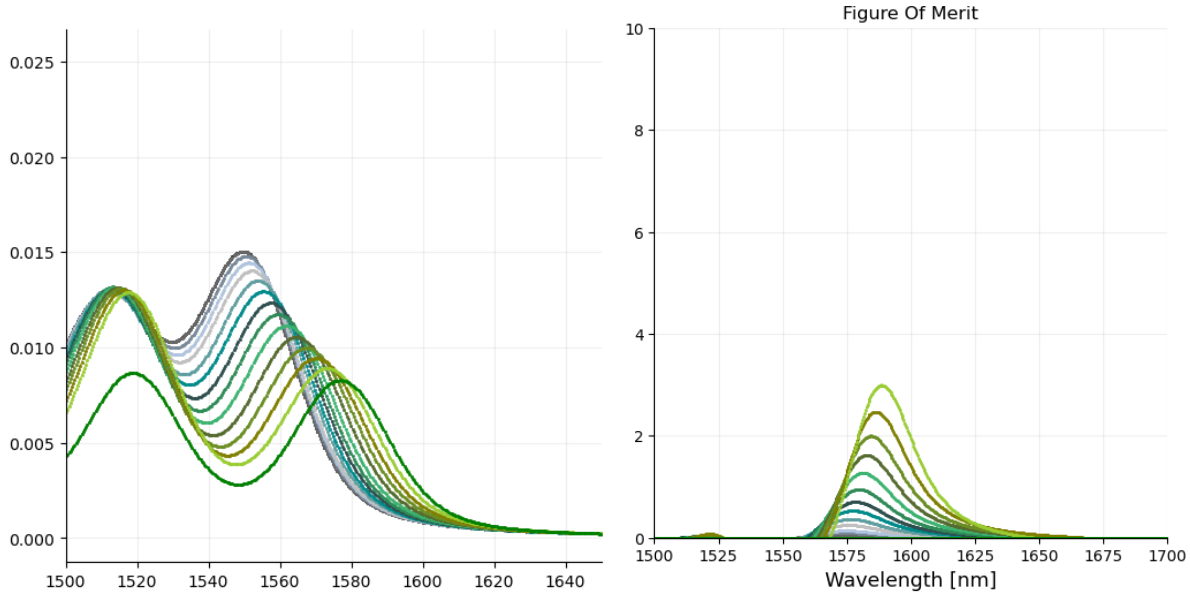
layer1 = Layer(InGaAlAs_material(1650.85), 100)

layer2 = Layer(InGaAlAs_material(1239.85), 100)

layer3 = Layer(InGaAlAs_material(1239.85), 100)

layers = [InP_layer2, layer1, InP_layer2]

Square well with high barriers:



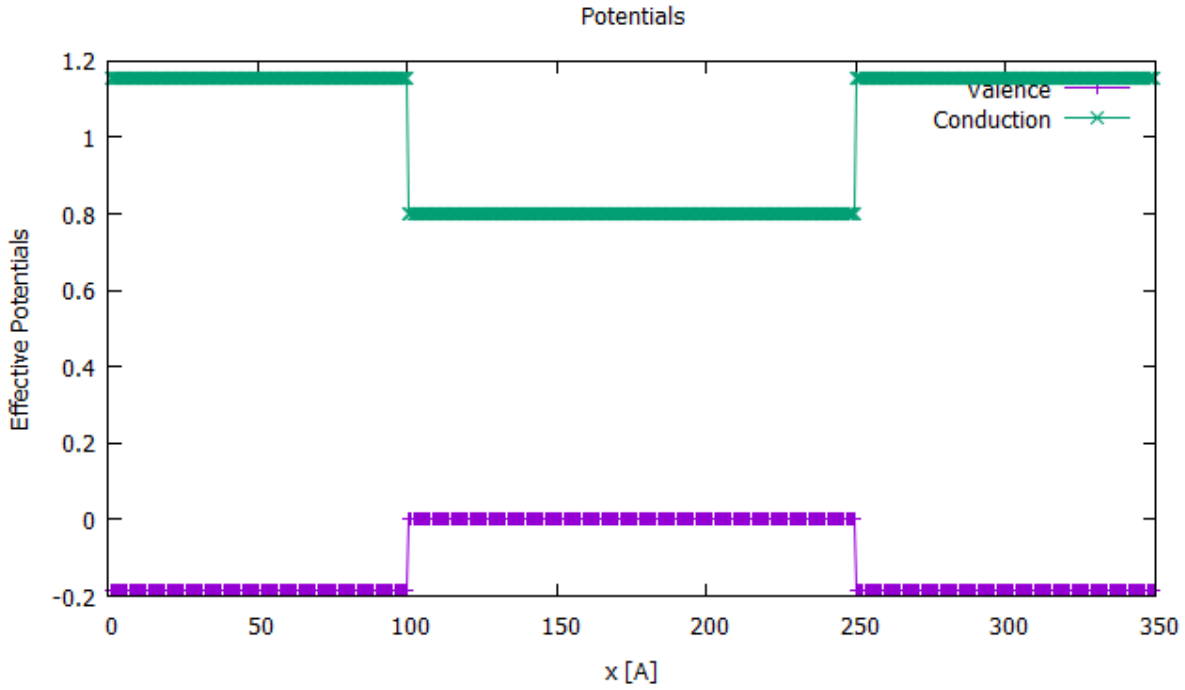
InP_layer2 = Layer(InGaAlAs_material(1039.85), 100)

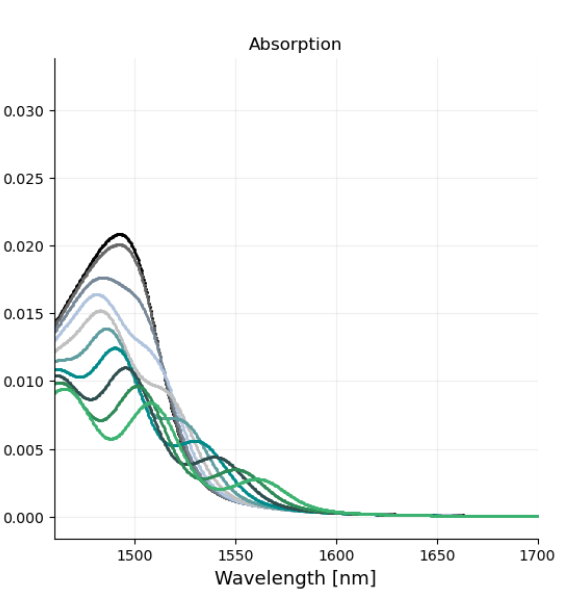
layer1 = Layer(InGaAlAs_material(1650.85), 150)

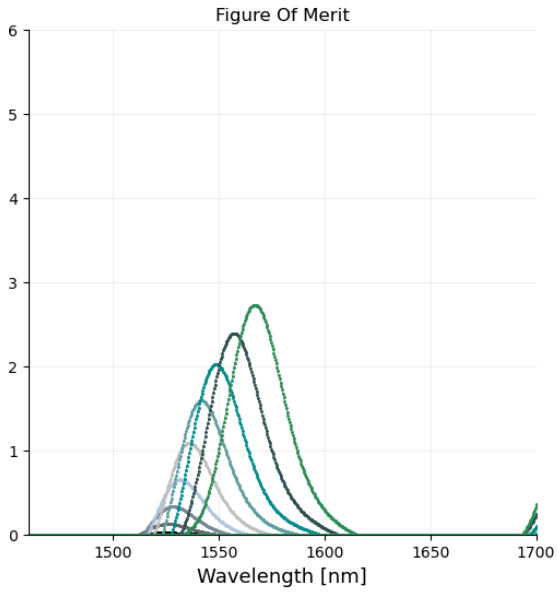
layer2 = Layer(InGaAlAs_material(1450.85), 50)

layer3 = Layer(InGaAlAs_material(1239.85), 50)

layers = [InP_layer2, layer1, InP_layer2]







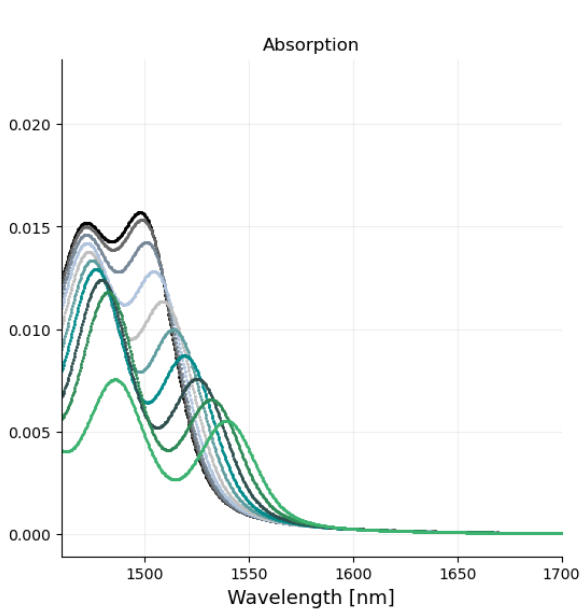
InP_layer2 = Layer(InGaAlAs_material(1039.85), 100)

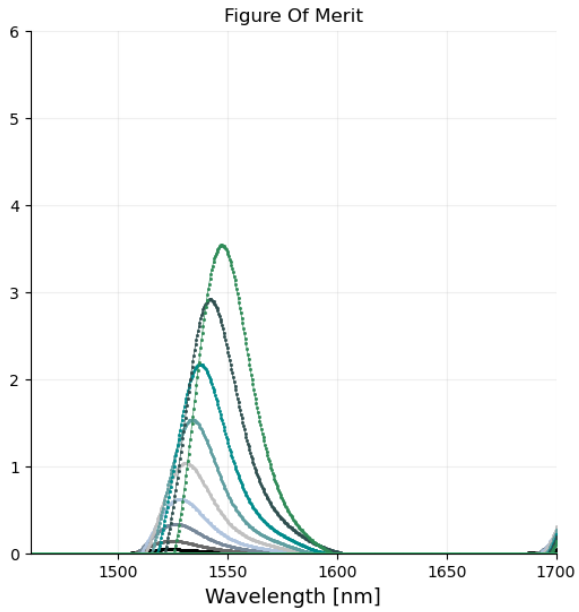
layer1 = Layer(InGaAlAs_material(1650.85), 100)

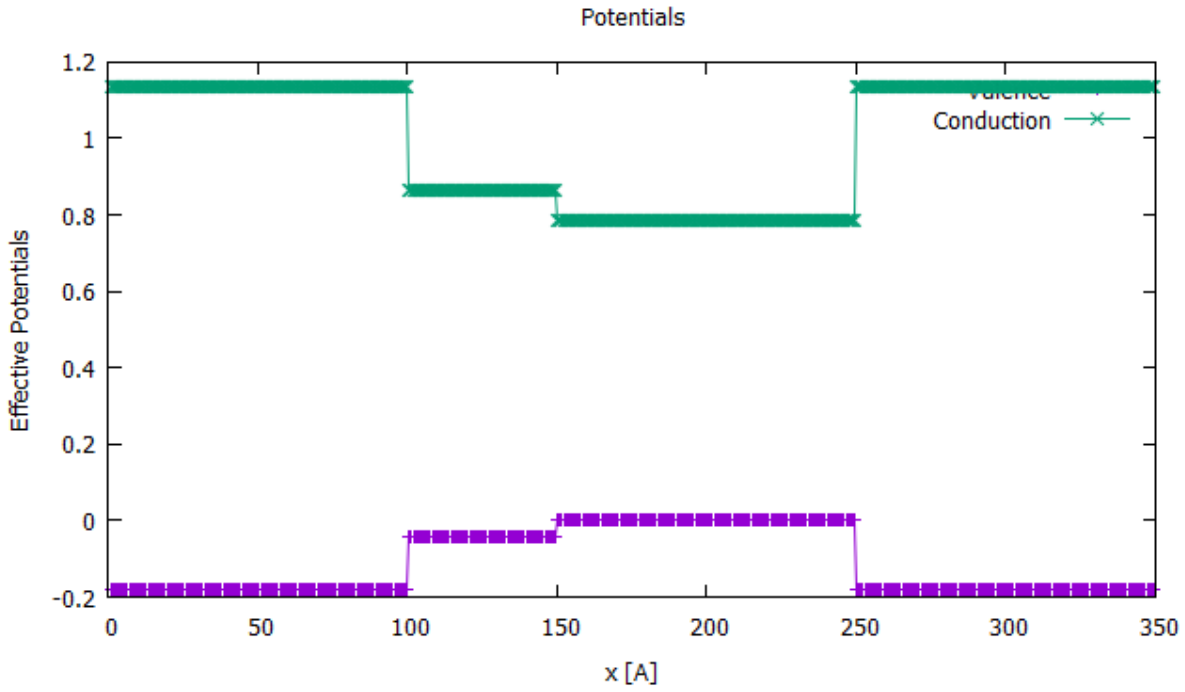
layer2 = Layer(InGaAlAs_material(1450.85), 50)

layer3 = Layer(InGaAlAs_material(1239.85), 50)

layers = [InP_layer2, layer2, layer1, InP_layer2]







InP_layer2 = Layer(InGaAlAs_material(1039.85), 100)

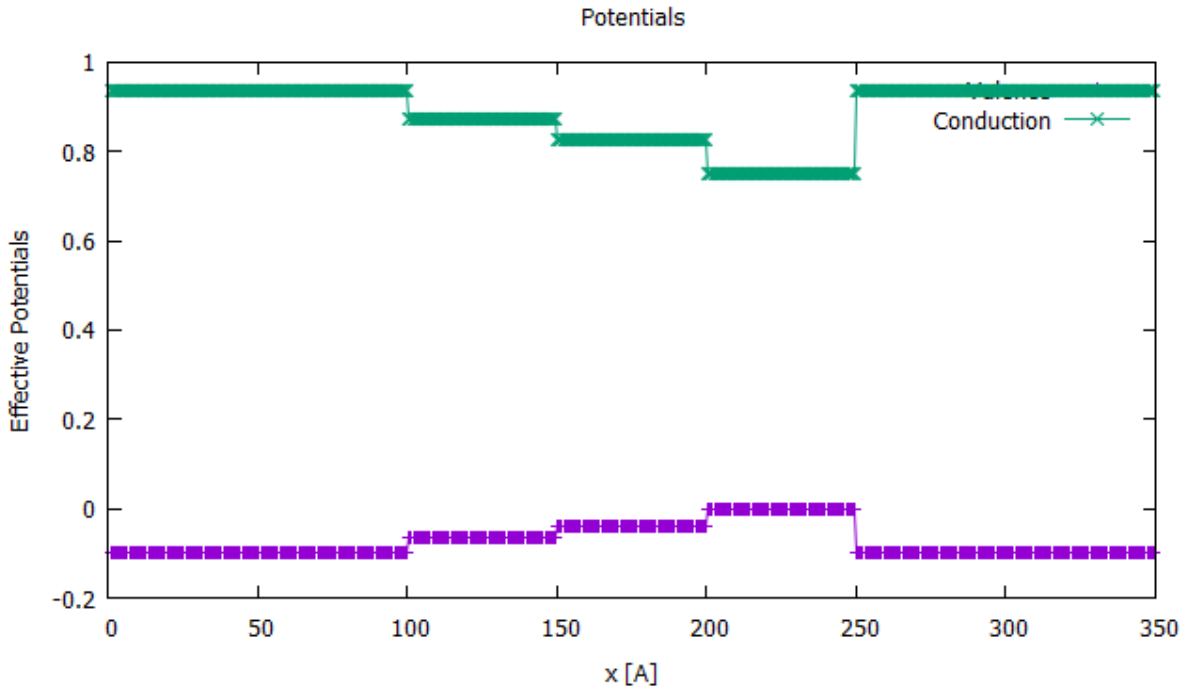
layer1 = Layer(InGaAlAs_material(1650.85), 50)

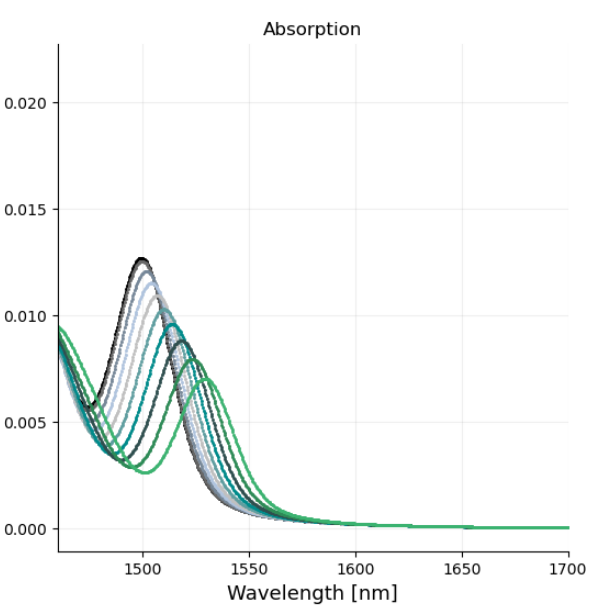
layer2 = Layer(InGaAlAs_material(1450.85), 50)

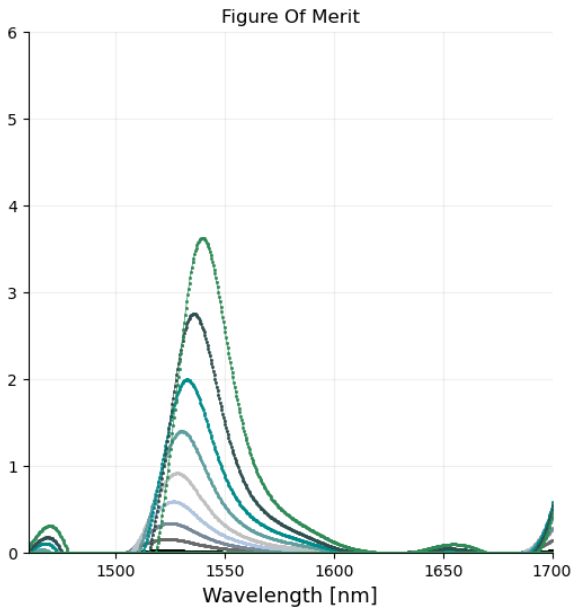
layer2 = Layer(InGaAlAs_material(1350.85), 50)

layer3 = Layer(InGaAlAs_material(1239.85), 50)

layers = [InP_layer2,layer3, layer2, layer1, InP_layer2]







InP_layer2 = Layer(InGaAlAs_material(1039.85), 100)

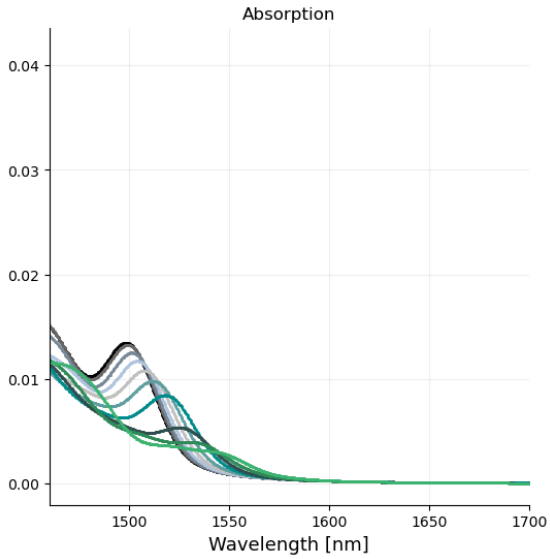
layer1 = Layer(InGaAlAs_material(1650.85), 30)

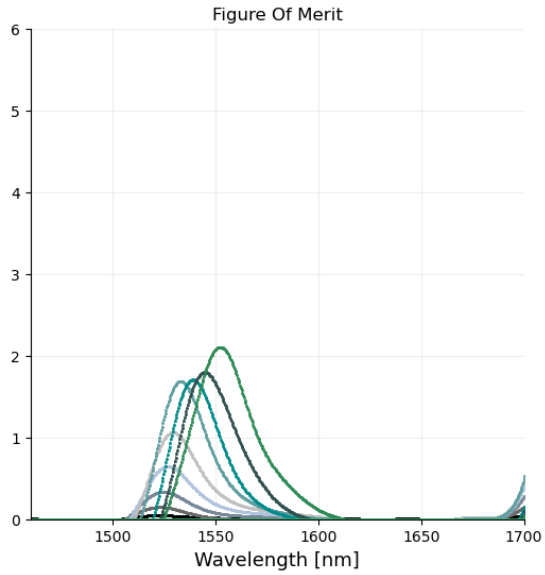
layer2 = Layer(InGaAlAs_material(1450.85), 30)

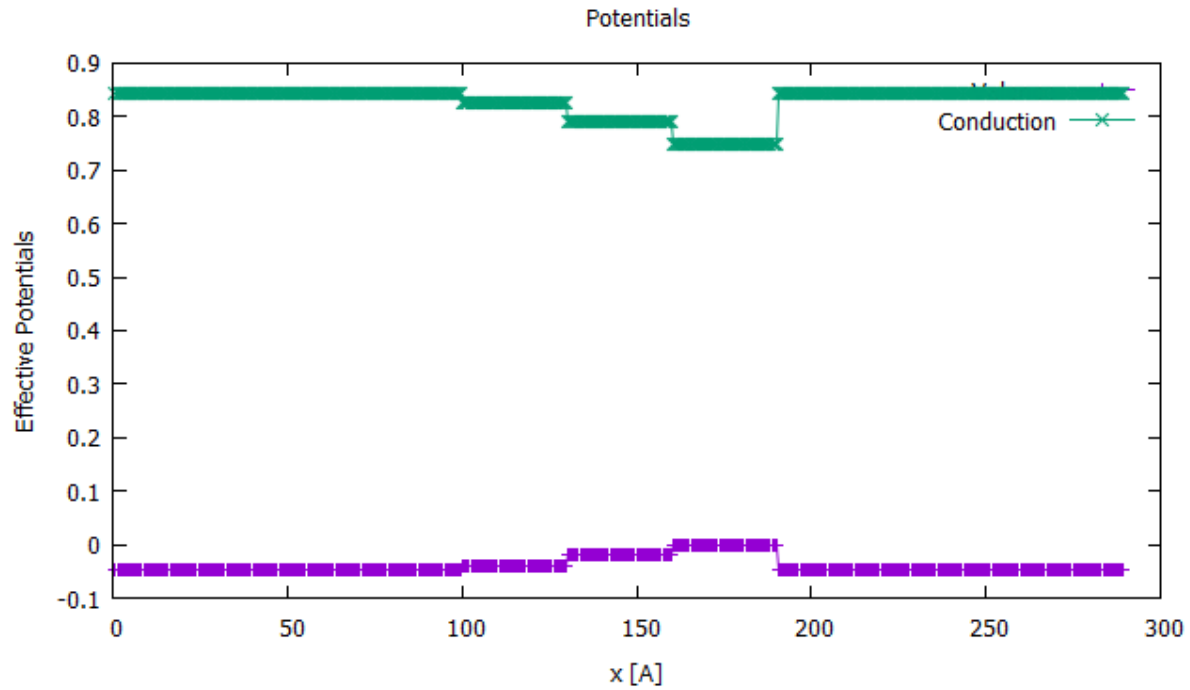
layer2 = Layer(InGaAlAs_material(1350.85), 30)

layer3 = Layer(InGaAlAs_material(1239.85), 30)

layers = [InP_layer2,layer3, layer2, layer1, InP_layer2]







InP_layer2 = Layer(InGaAlAs_material(1039.85), 100)

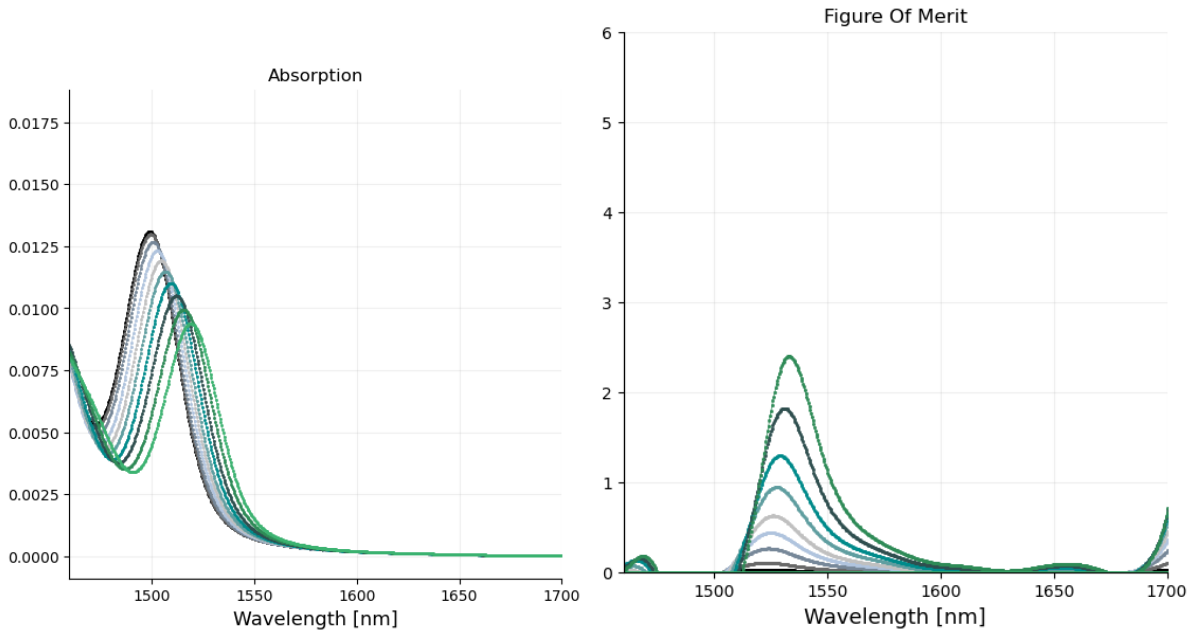
layer1 = Layer(InGaAlAs_material(1650.85), 50)

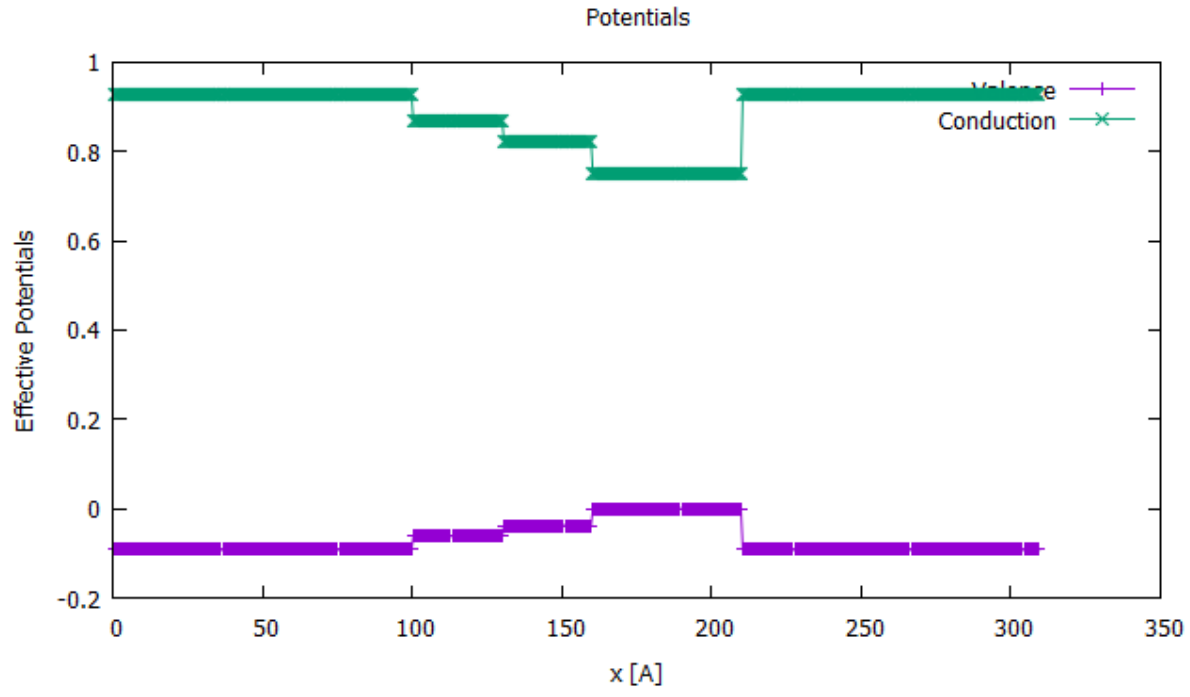
layer2 = Layer(InGaAlAs_material(1450.85), 30)

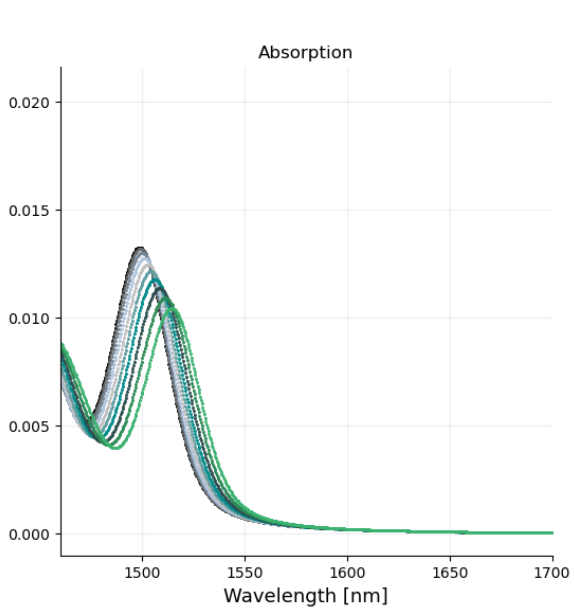
layer2 = Layer(InGaAlAs_material(1350.85), 30)

layer3 = Layer(InGaAlAs_material(1239.85), 30)

layers = [InP_layer2,layer3, layer2, layer1, InP_layer2]






Absorption
0.020
0.015
0.010
0.005
0.000
1500
1550
1600
1650
1700
Wavelength [nm]

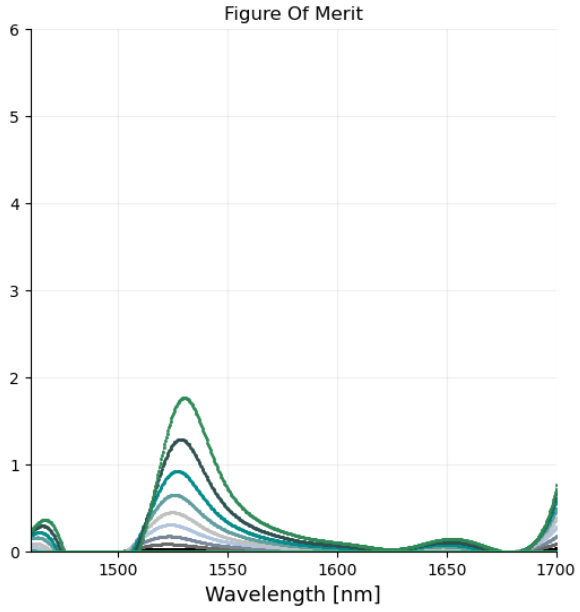
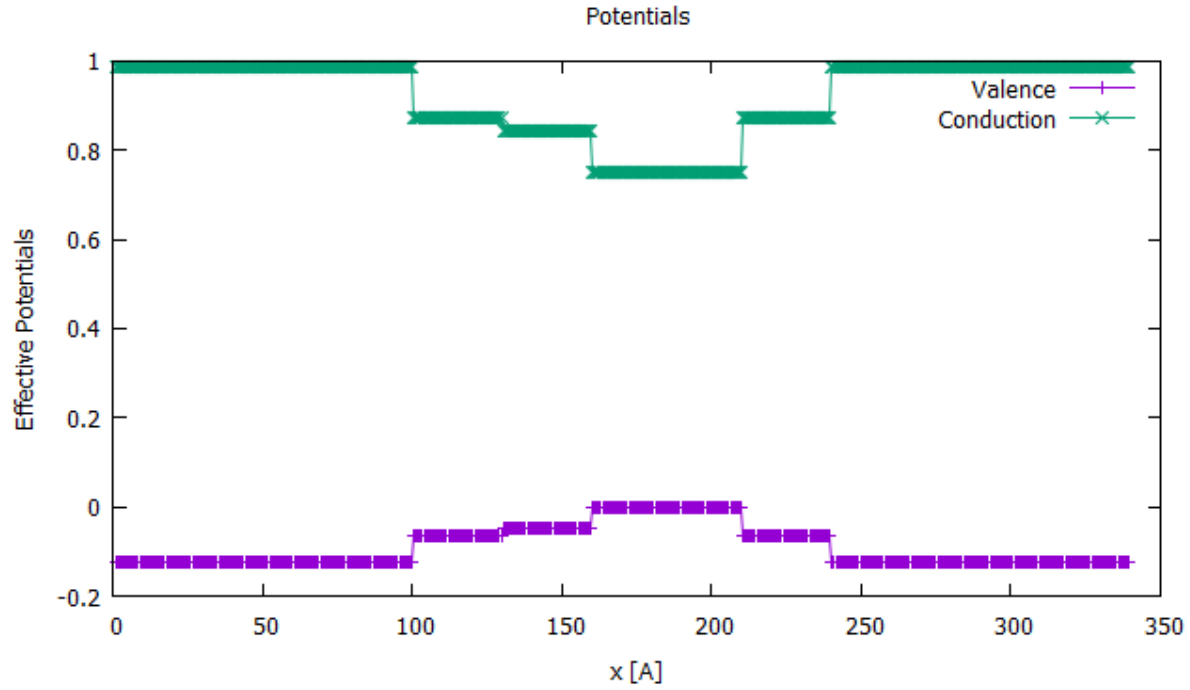


Figure Of Merit
6
5
4
3
2
1
0
1500
1550
1600
1650
1700
Wavelength [nm]


Potentials
Valence
Conduction
Effective Potentials
1
0.8
0.6
0.4
0.2
0
-0.2
0
50
100
150
200
250
300
350
x [A]

InP_layer2 = Layer(InGaAlAs_material(1039.85), 100)

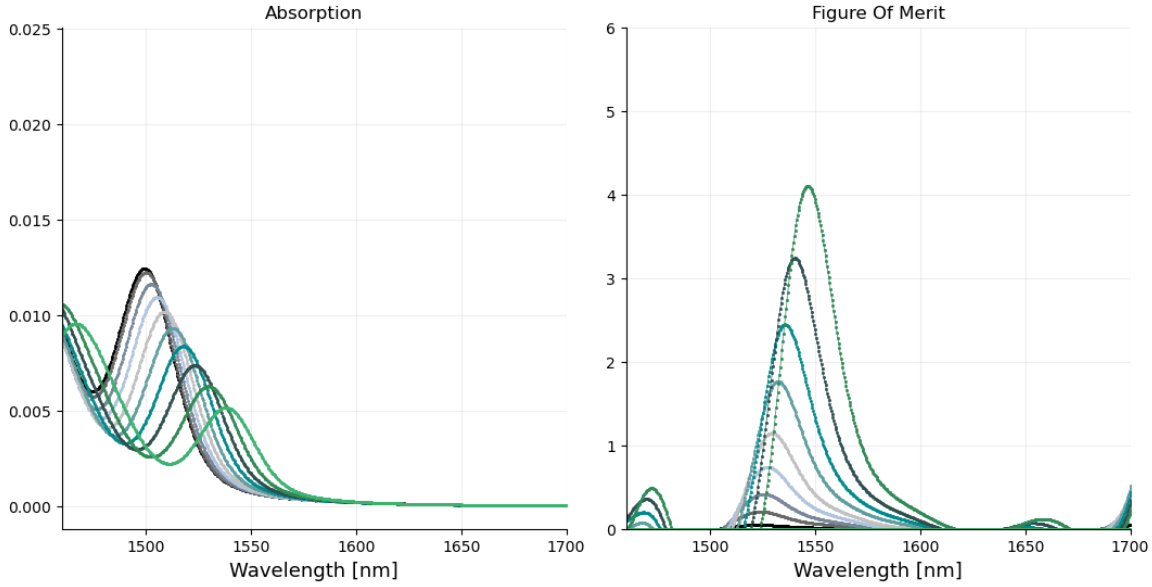
layer1 = Layer(InGaAlAs_material(1650.85), 50)

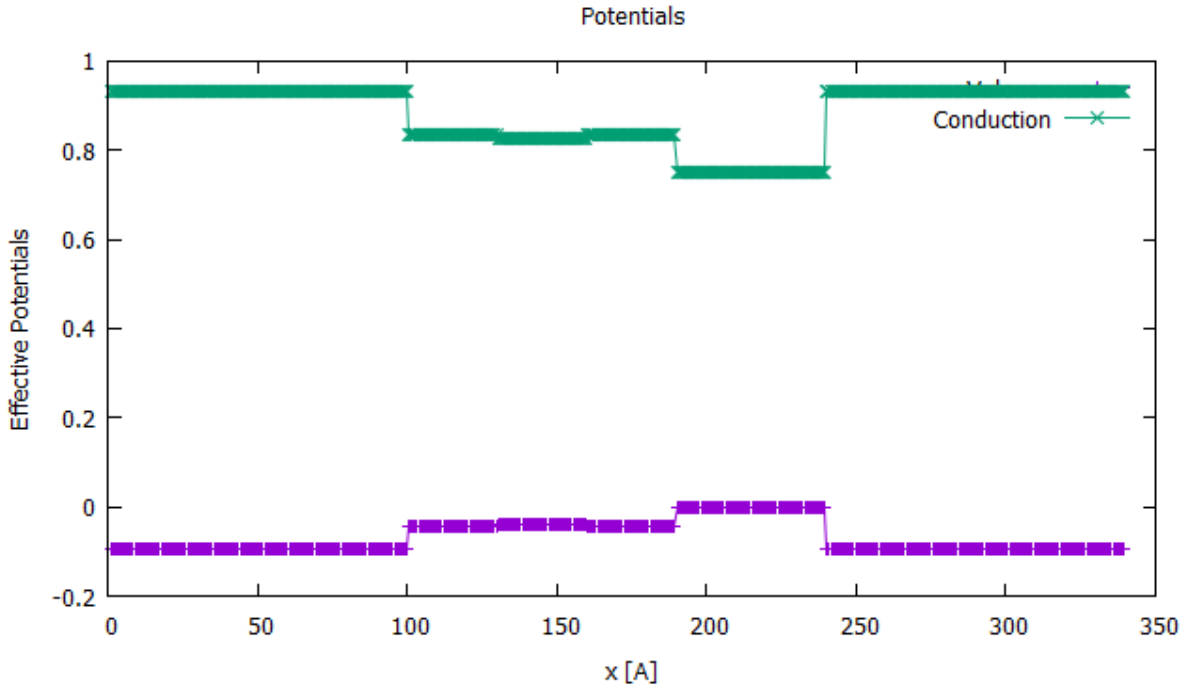
layer2 = Layer(InGaAlAs_material(1450.85), 30)

layer2 = Layer(InGaAlAs_material(1350.85), 30)

layer3 = Layer(InGaAlAs_material(1239.85), 30)

layers = [InP_layer2, layer3, layer2, layer3, layer1, InP_layer2]





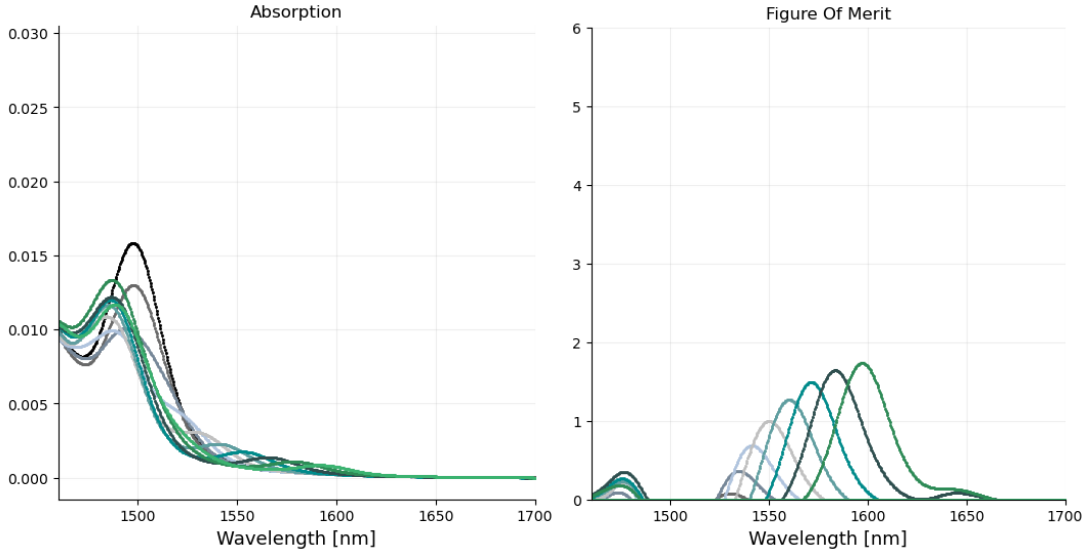
InP_layer2 = Layer(InGaAlAs_material(1039.85), 100)

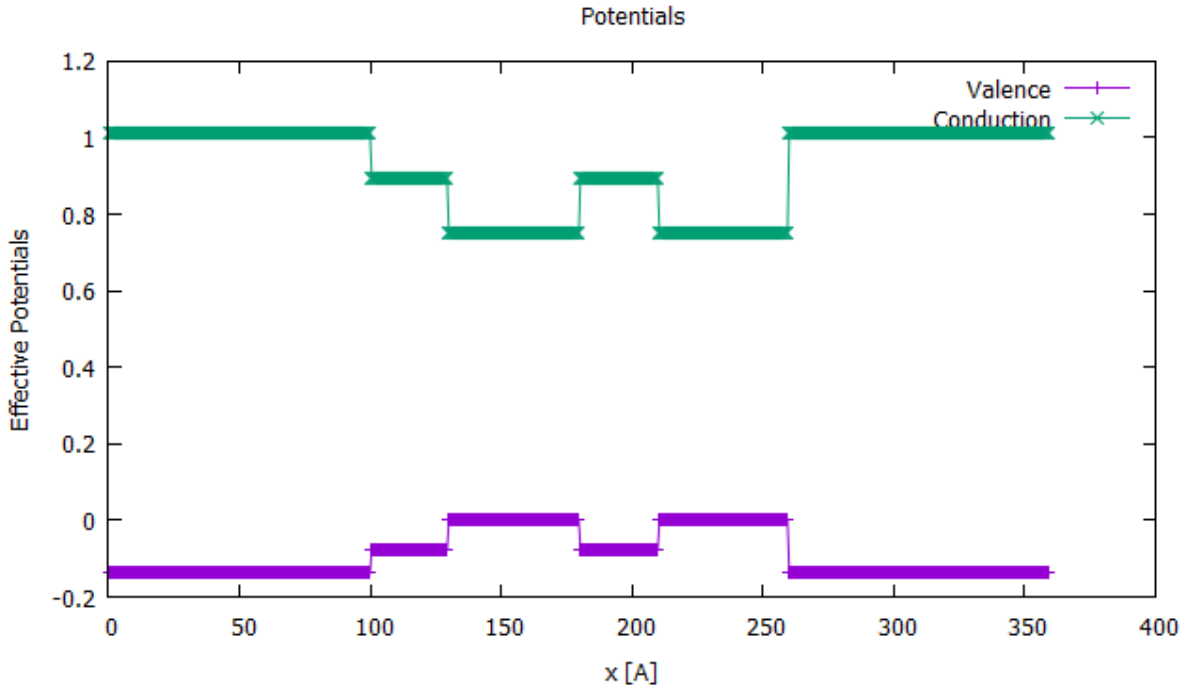
layer1 = Layer(InGaAlAs_material(1650.85), 50)

layer2 = Layer(InGaAlAs_material(1450.85), 30)

layer2 = Layer(InGaAlAs_material(1350.85), 30)

layer3 = Layer(InGaAlAs_material(1239.85), 30)





InP_layer2 = Layer(InGaAlAs_material(1039.85), 100)

layer1 = Layer(InGaAlAs_material(1650.85), 50)

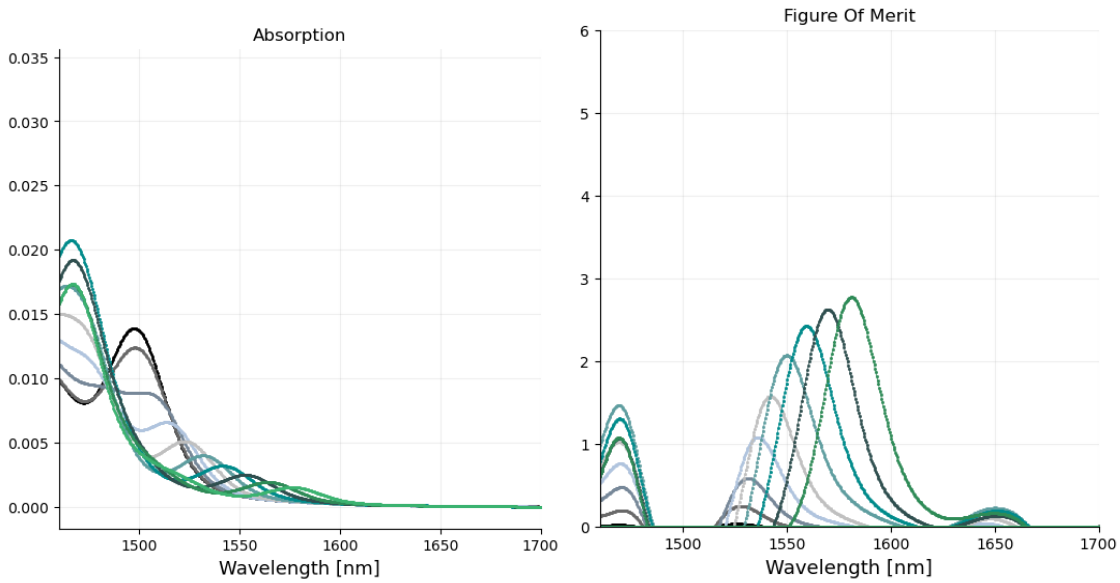
layer2 = Layer(InGaAlAs_material(1450.85), 30)

layer2 = Layer(InGaAlAs_material(1350.85), 30)

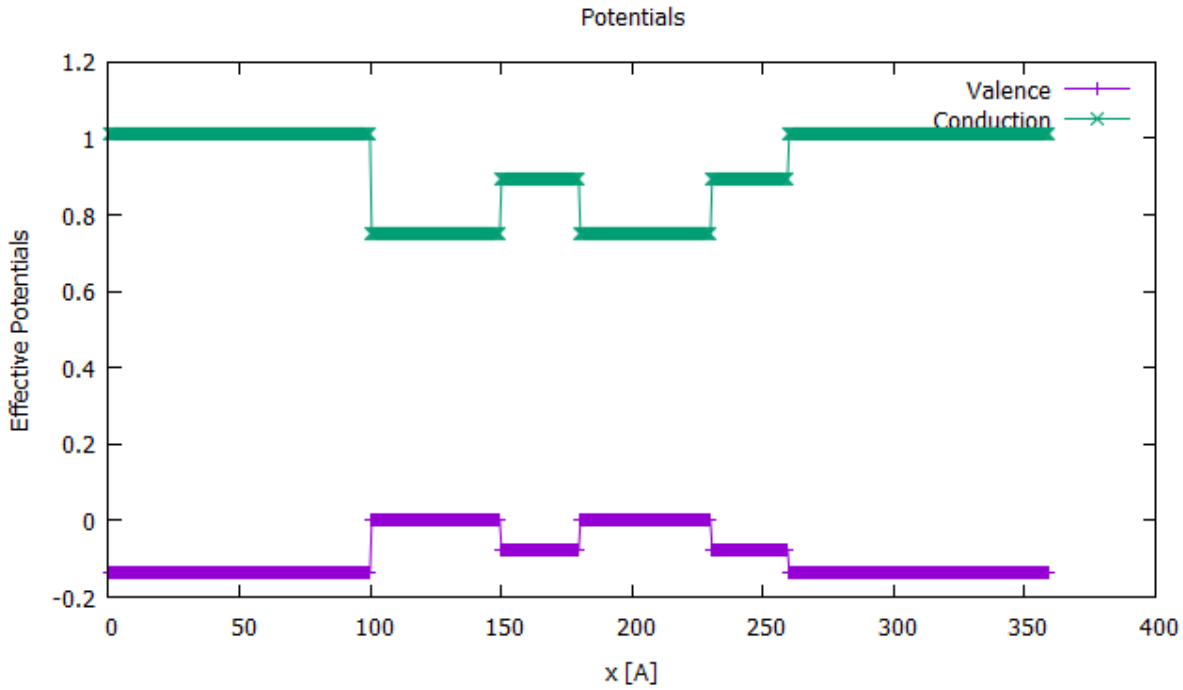
layer3 = Layer(InGaAlAs_material(1239.85), 30)

layer4 = Layer(InGaAlAs_material(1239.85), 30)

layers = [InP_layer2, layer1, layer3, layer1, layer3, InP_layer2]



Interesting because theres a possibility for inverted operation principle?



InP_layer2 = Layer(InGaAlAs_material(1039.85), 100)

layer1 = Layer(InGaAlAs_material(1650.85), 50)

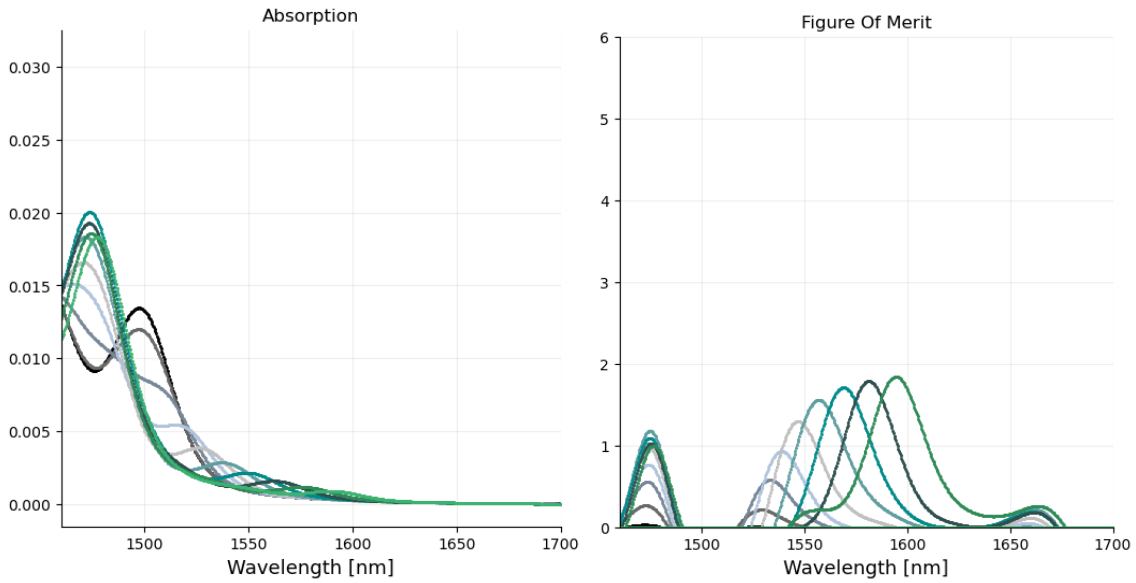
layer2 = Layer(InGaAlAs_material(1450.85), 30)

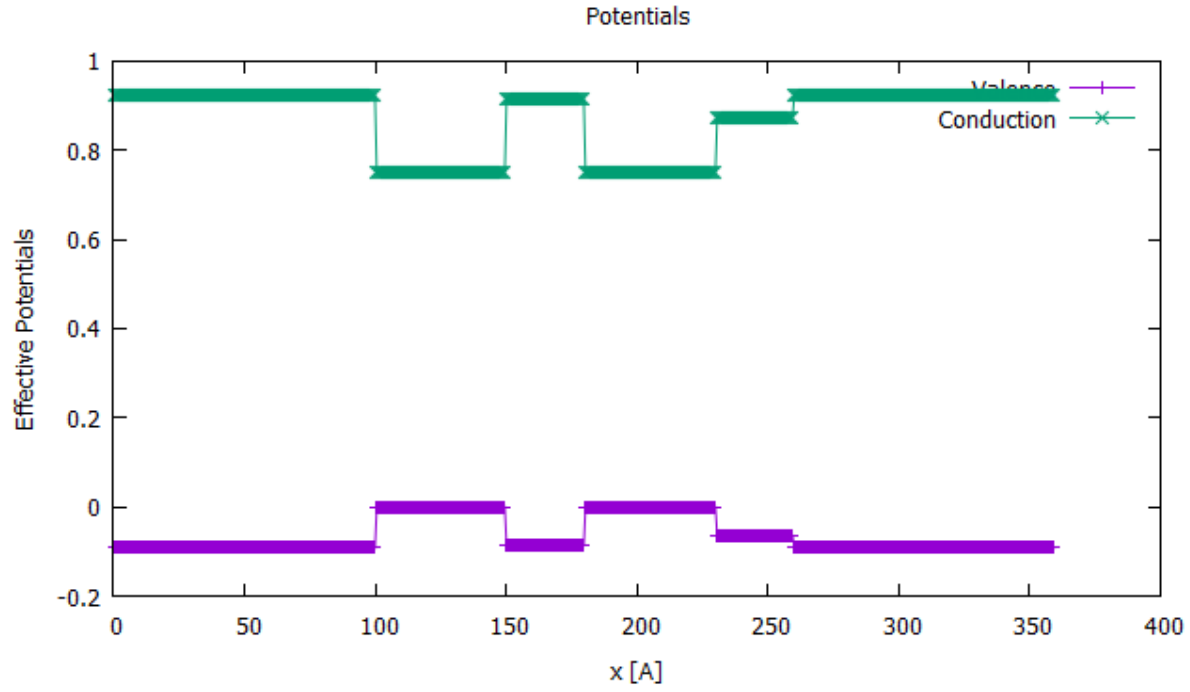
layer2 = Layer(InGaAlAs_material(1350.85), 30)

layer3 = Layer(InGaAlAs_material(1239.85), 30)

layer4 = Layer(InGaAlAs_material(1139.85), 30)

layers = [InP_layer2, layer1, layer4, layer1, layer3, InP_layer2]





InP_layer2 = Layer(InGaAlAs_material(1039.85), 100)

layer1 = Layer(InGaAlAs_material(1650.85), 50)

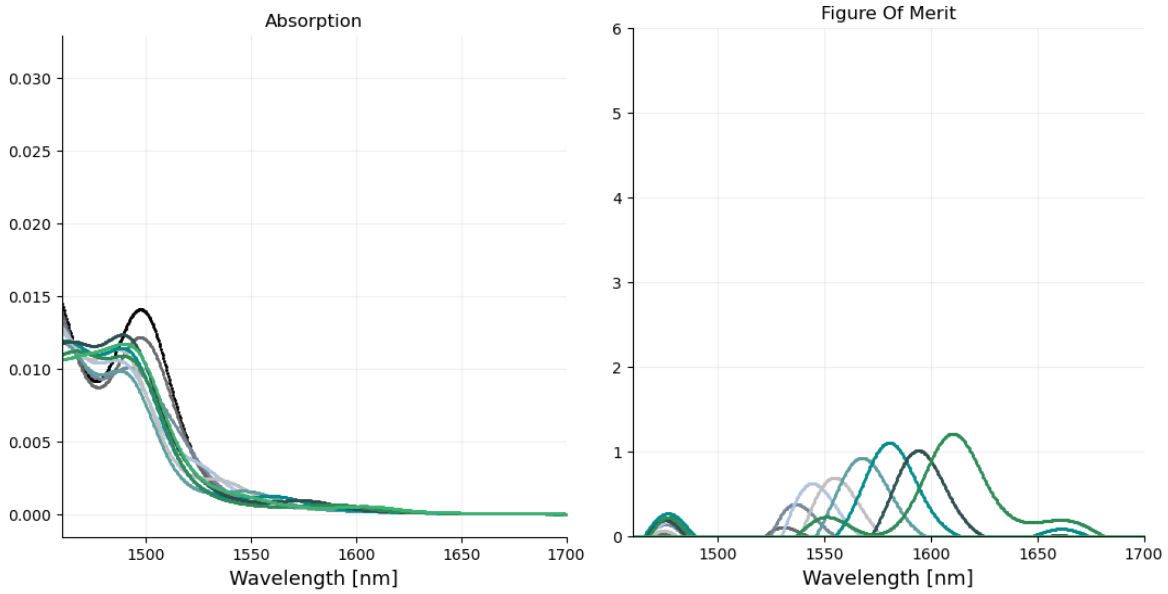
layer2 = Layer(InGaAlAs_material(1450.85), 30)

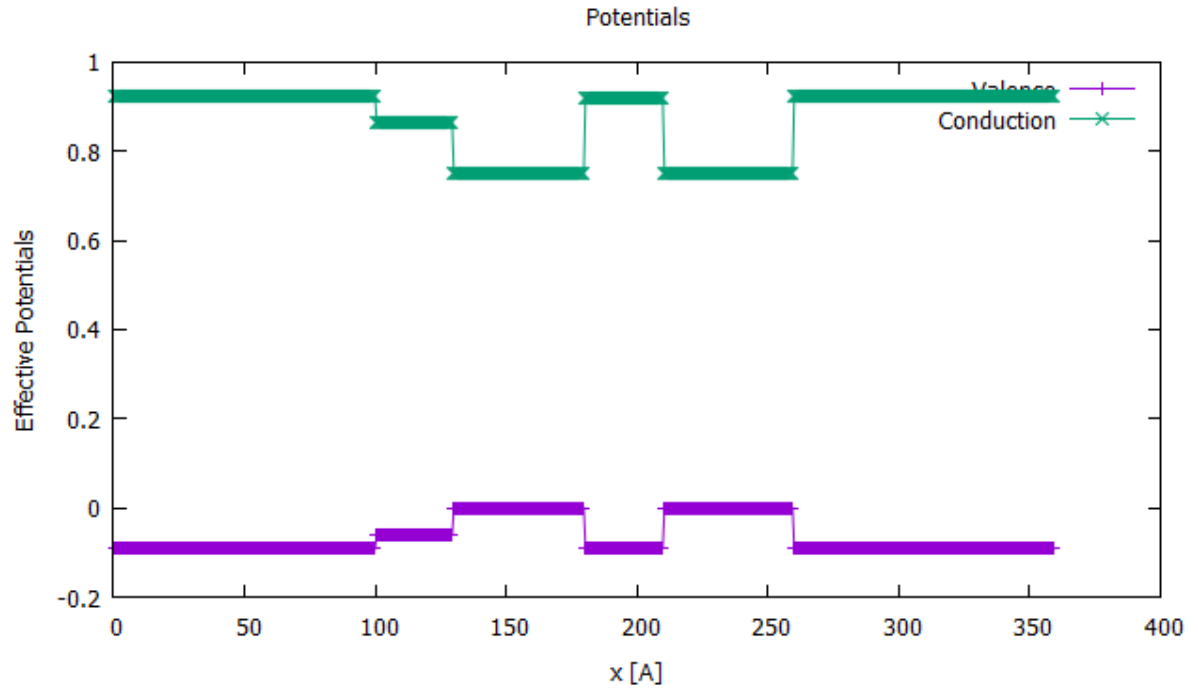
layer2 = Layer(InGaAlAs_material(1350.85), 30)

layer3 = Layer(InGaAlAs_material(1239.85), 30)

layer4 = Layer(InGaAlAs_material(1139.85), 30)

layers = [InP_layer2,layer3, layer1, layer4, layer1, InP_layer2]





InP_layer2 = Layer(InGaAlAs_material(1039.85), 100)

layer1 = Layer(InGaAlAs_material(1650.85), 60)

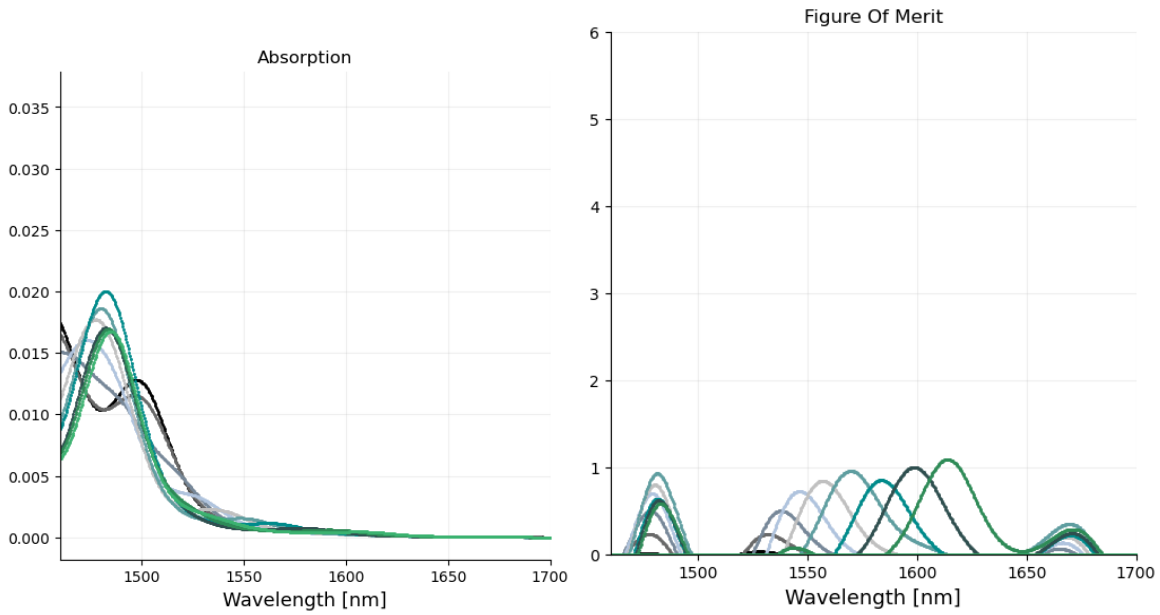
layer2 = Layer(InGaAlAs_material(1450.85), 30)

layer2 = Layer(InGaAlAs_material(1350.85), 30)

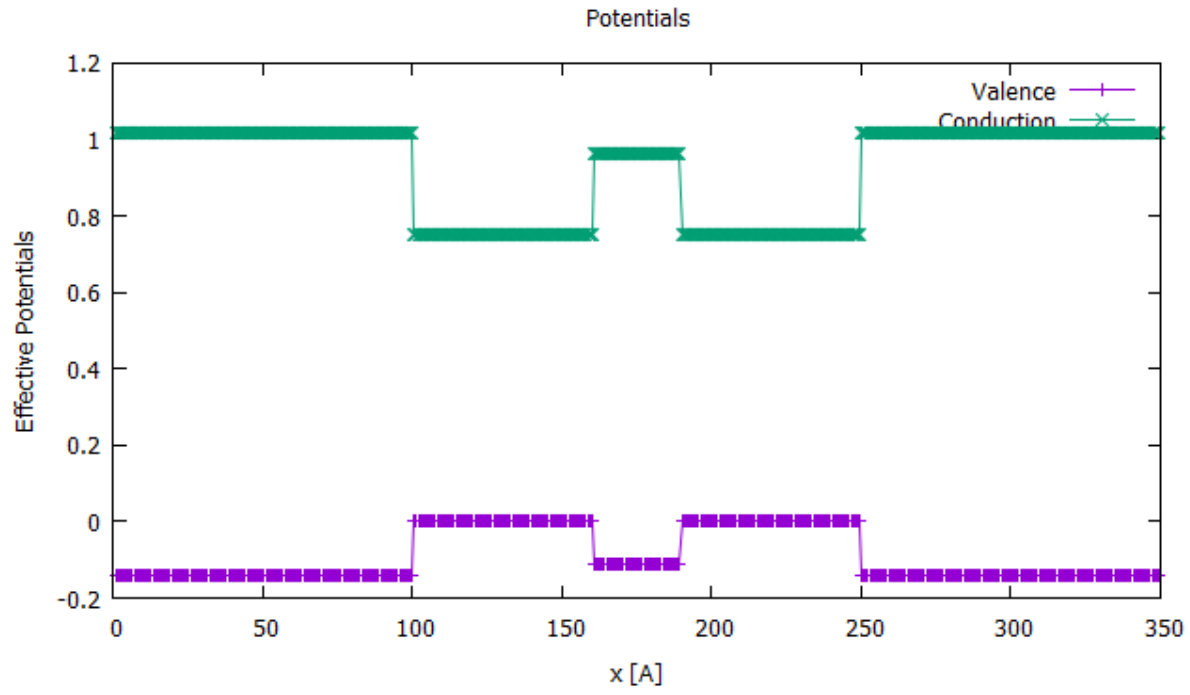
layer3 = Layer(InGaAlAs_material(1239.85), 30)

layer4 = Layer(InGaAlAs_material(1139.85), 30)

layers = [InP_layer2, layer1, layer4, layer1, InP_layer2]



Doesn't work so well for larger well regions



InP_layer2 = Layer(InGaAlAs_material(1039.85), 100)

layer1 = Layer(InGaAlAs_material(1650.85), 30)

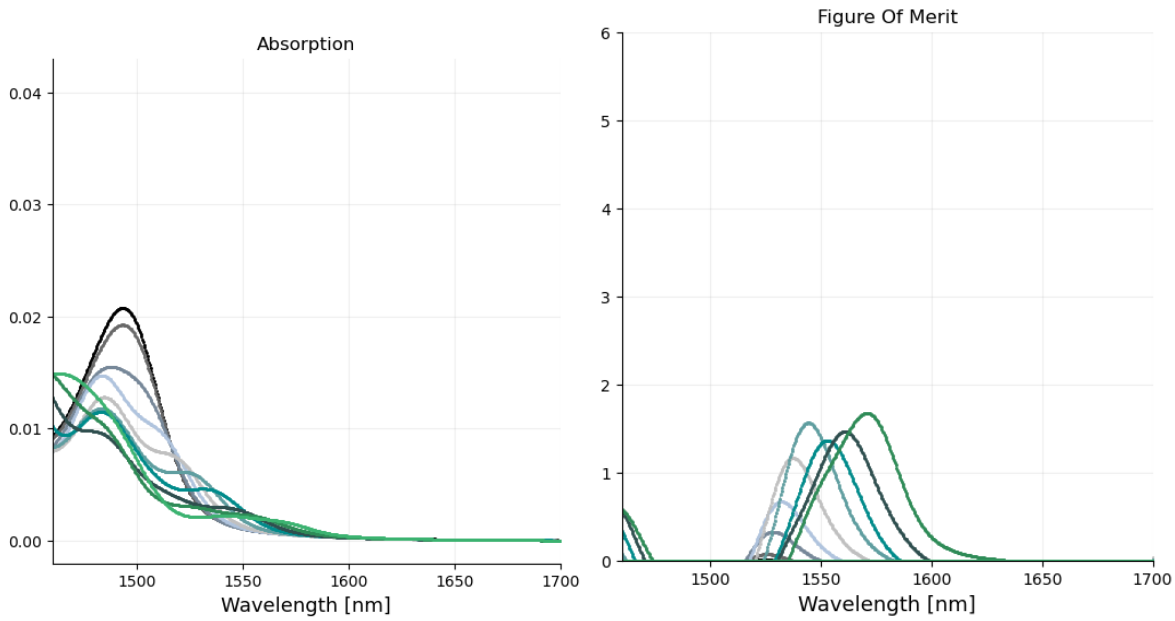
layer2 = Layer(InGaAlAs_material(1450.85), 30)

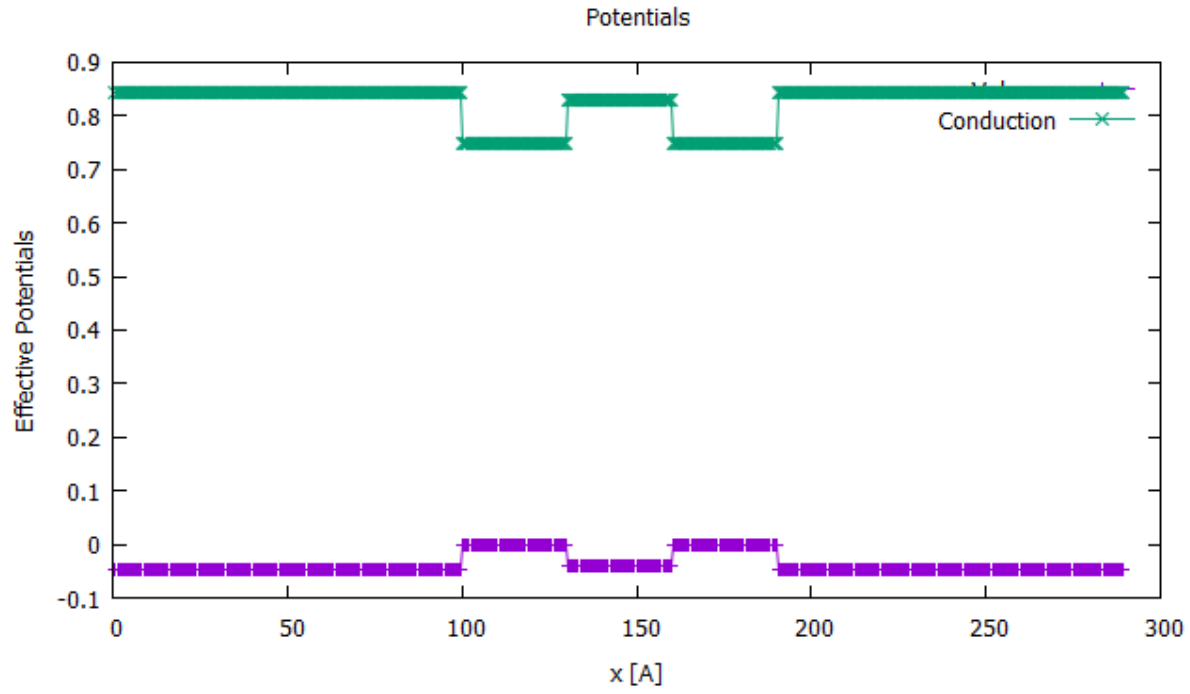
layer2 = Layer(InGaAlAs_material(1350.85), 30)

layer3 = Layer(InGaAlAs_material(1239.85), 30)

layer4 = Layer(InGaAlAs_material(1239.85), 30)

layers = [InP_layer2, layer1, layer4, layer1, InP_layer2]





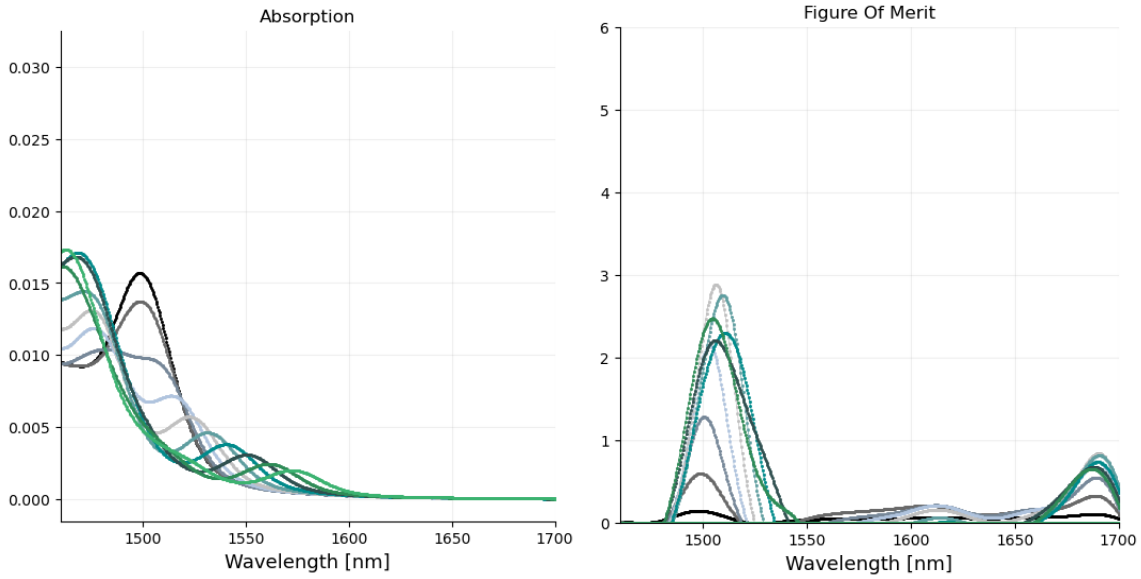


Figure of merit with “on”/”off” switched places

InP_layer2 = Layer(InGaAlAs_material(1039.85), 100)

layer1 = Layer(InGaAlAs_material(1650.85), 50)

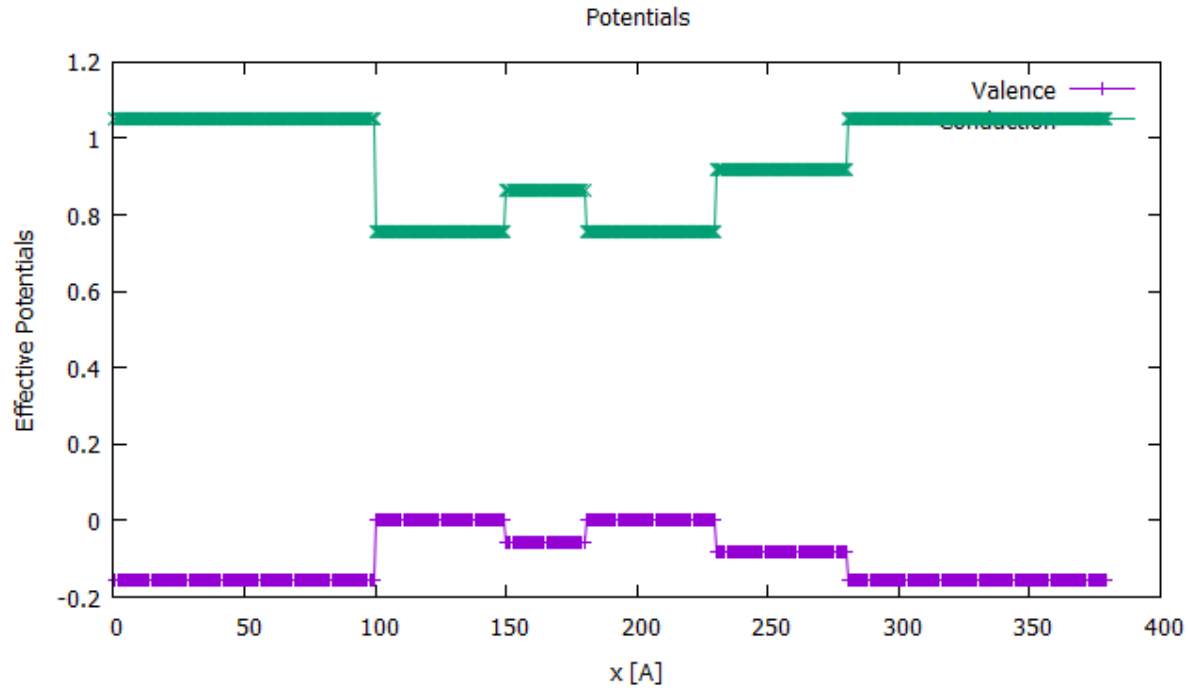
layer2 = Layer(InGaAlAs_material(1450.85), 30)

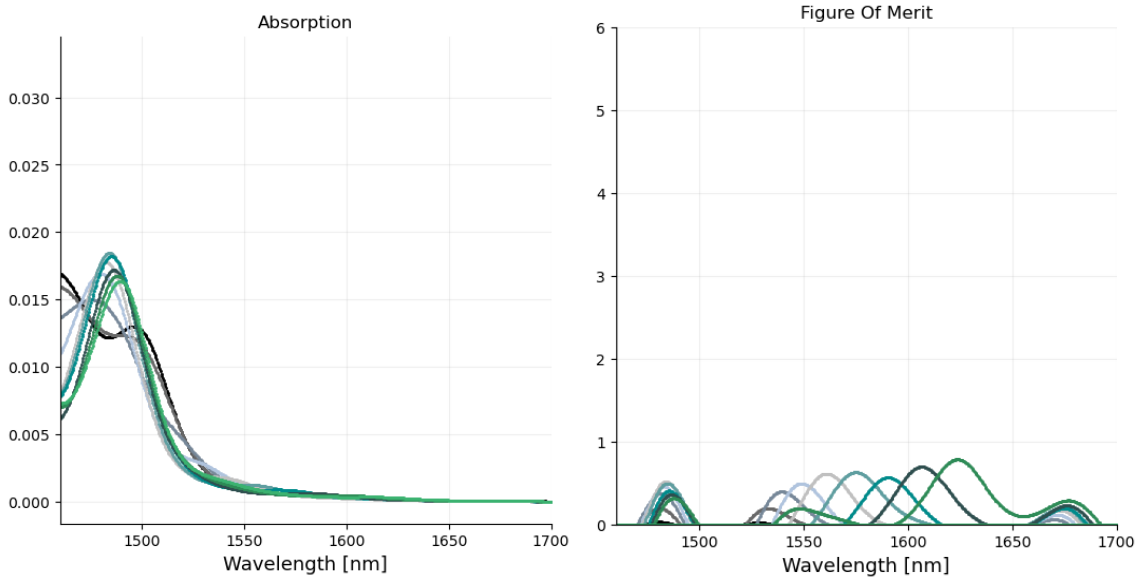
layer2 = Layer(InGaAlAs_material(1350.85), 30)

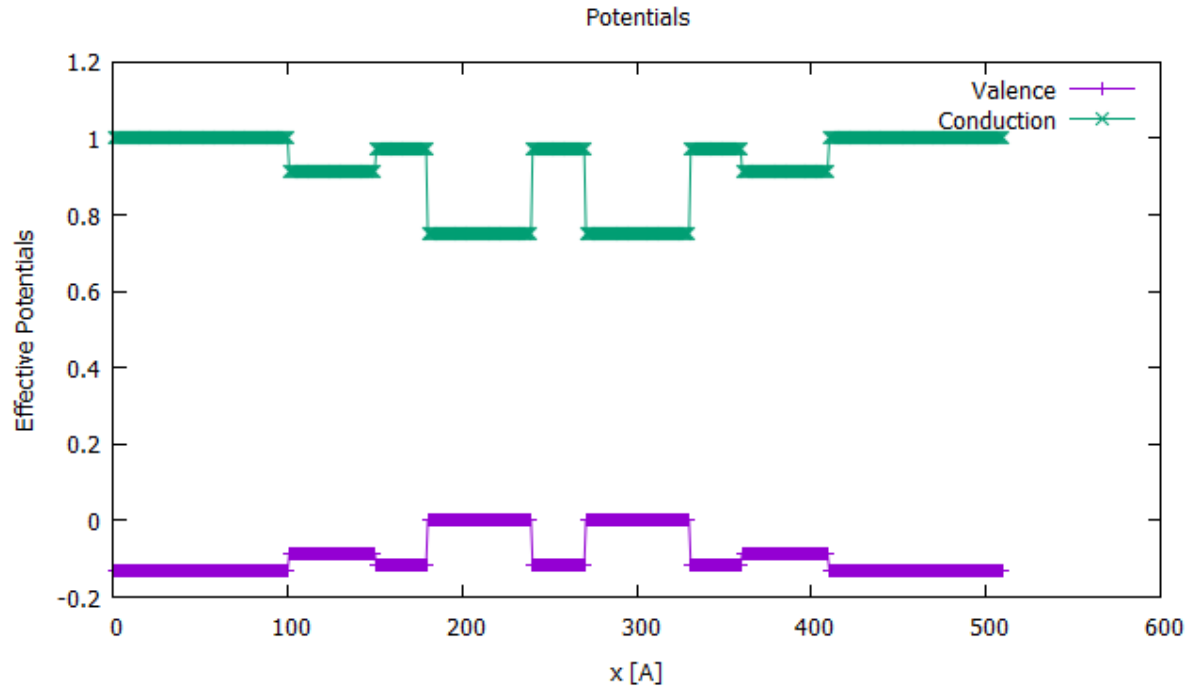
layer3 = Layer(InGaAlAs_material(1239.85), 50)

layer4 = Layer(InGaAlAs_material(1139.85), 30)

layers = [InP_layer2, layer1, layer2, layer1, layer3, InP_layer2]







InP_layer2 = Layer(InGaAlAs_material(1039.85), 100)

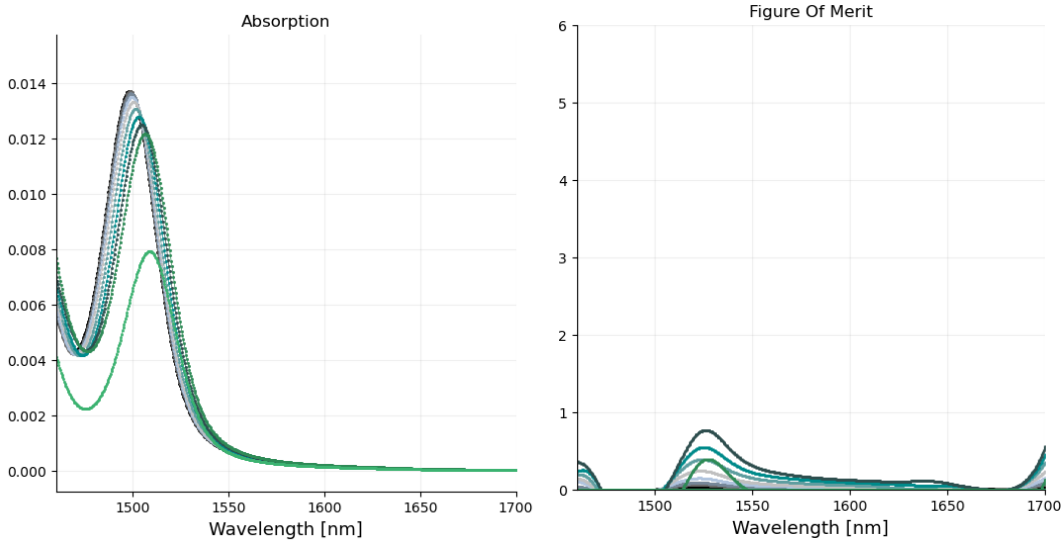
layer1 = Layer(InGaAlAs_material(1650.85), 60)

layer2 = Layer(InGaAlAs_material(1050.85), 30)

layer3 = Layer(InGaAlAs_material(1190.85), 50)

layer4 = Layer(InGaAlAs_material(1139.85), 30)

layers = [InP_layer2,layer3,layer2, layer1, layer2, layer1,layer2, layer3, InP_layer2]



InP_layer2 = Layer(InGaAlAs_material(1039.85), 100)

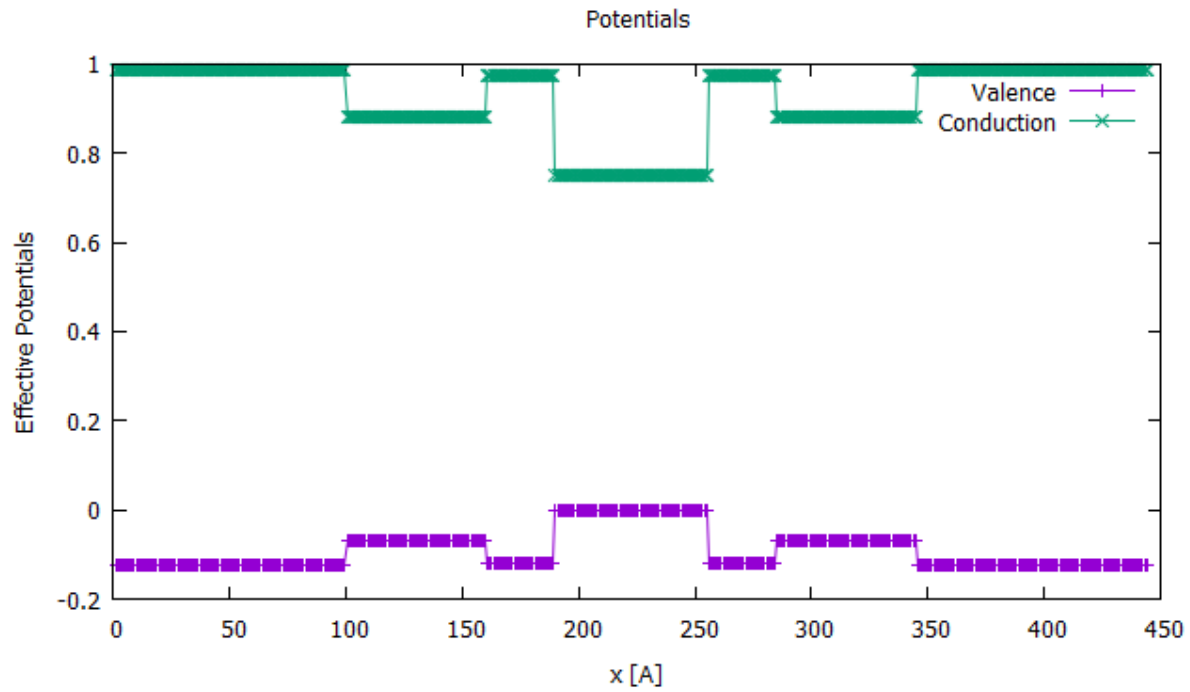
layer1 = Layer(InGaAlAs_material(1650.85), 65)

layer2 = Layer(InGaAlAs_material(1050.85), 30)

layer3 = Layer(InGaAlAs_material(1230.85), 60)

layer4 = Layer(InGaAlAs_material(1139.85), 30)

layers = [InP_layer2,layer3,layer2, layer1, layer2, layer3, InP_layer2]



InP_layer2 = Layer(InGaAlAs_material(1239.85), 100)

layer1 = Layer(InGaAlAs_material(1630.85), 50)

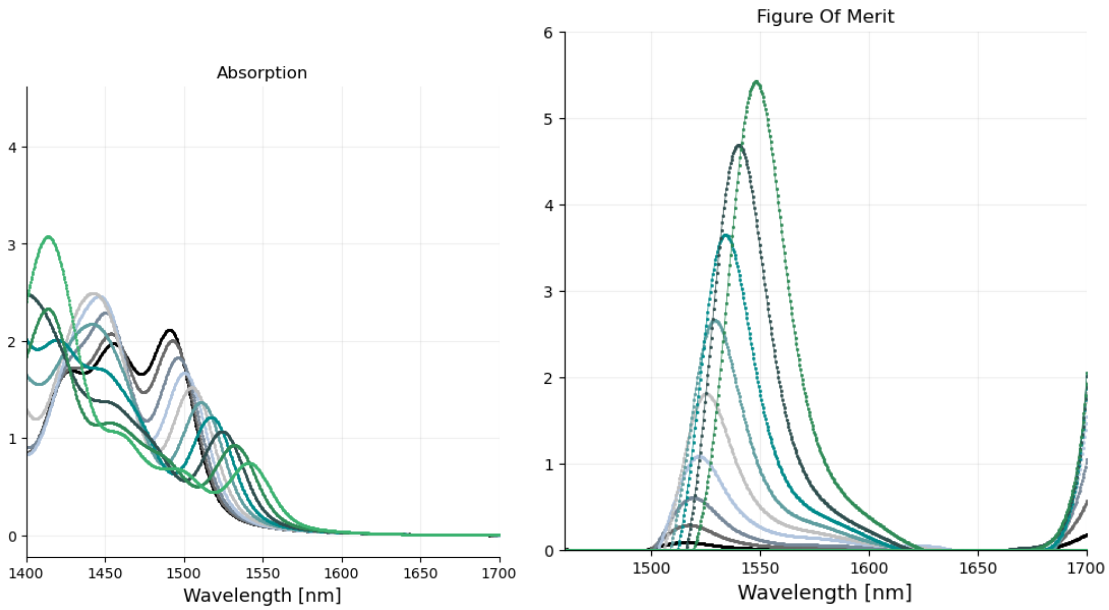
layer2 = Layer(InGaAlAs_material(1400.85), 30)

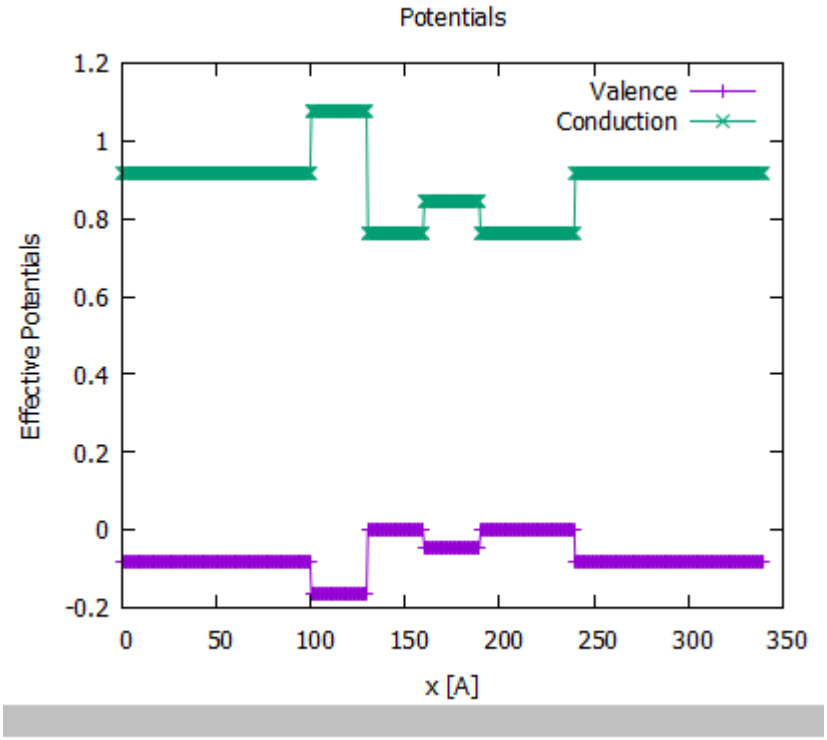
layer3 = Layer(InGaAlAs_material(1000.00), 30)

layer4 = Layer(InGaAlAs_material(1630.85), 30)

layers = [InP_layer2,layer3,layer4, layer2, layer1, InP_layer2]

```
Initial Bandgap: 1491.7544475937038
```





10 V/um

InP_layer2 = Layer(InGaAlAs_material(1239.85), 100)

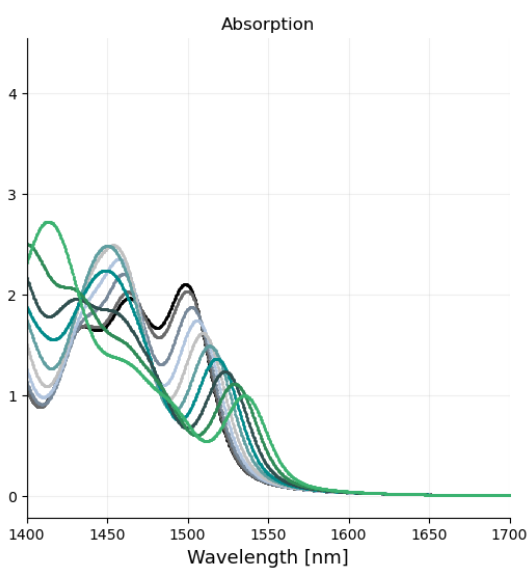
layer1 = Layer(InGaAlAs_material(1630.85), 50)

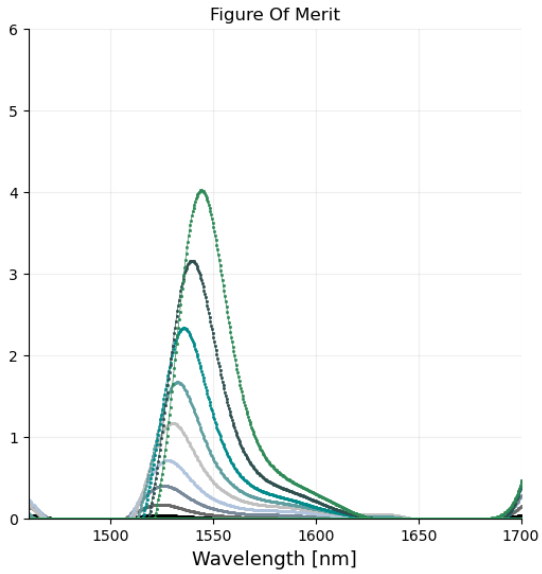
layer2 = Layer(InGaAlAs_material(1400.85), 30)

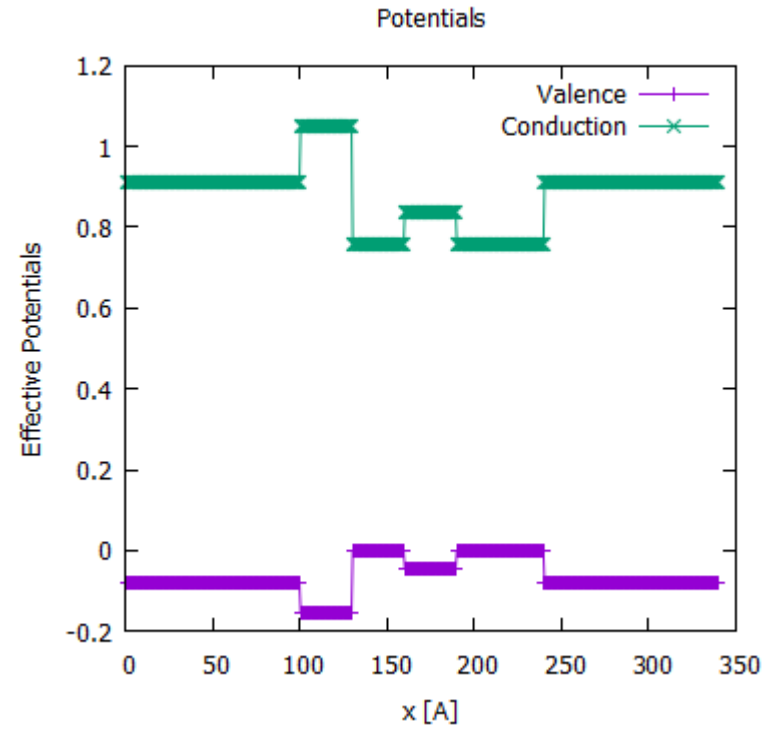
layer3 = Layer(InGaAlAs_material(1000.00), 30)

layer4 = Layer(InGaAlAs_material(1630.85), 30)

layers = [InP_layer2,layer3,layer4, layer2, layer1, InP_layer2]







InP_layer2 = Layer(InGaAlAs_material(1239.85), 100)

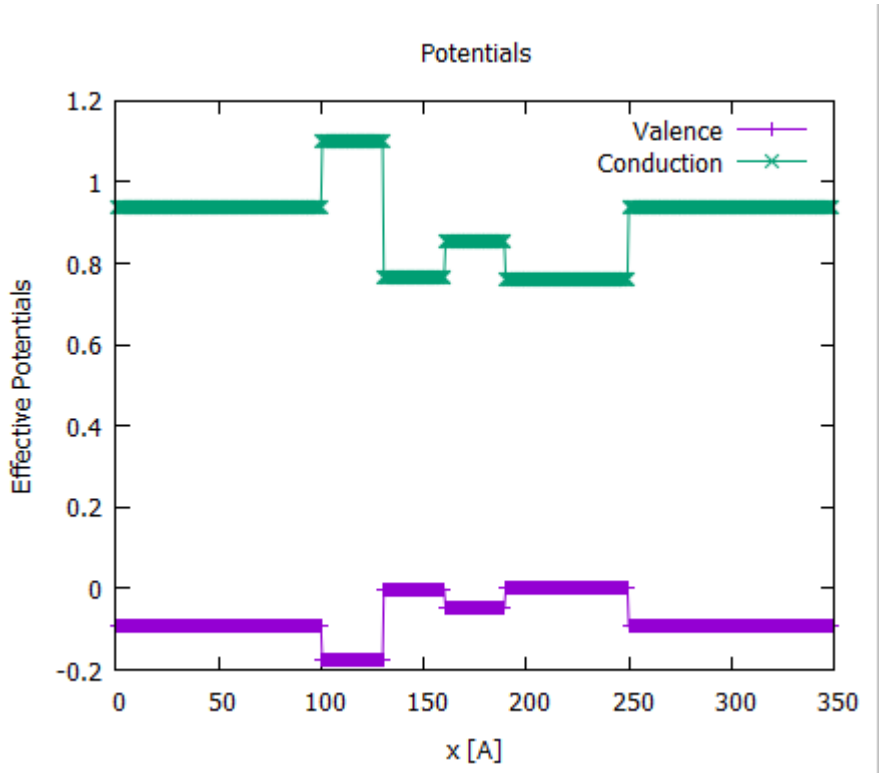
layer1 = Layer(InGaAlAs_material(1650.85), 60)

layer2 = Layer(InGaAlAs_material(1400.85), 30)

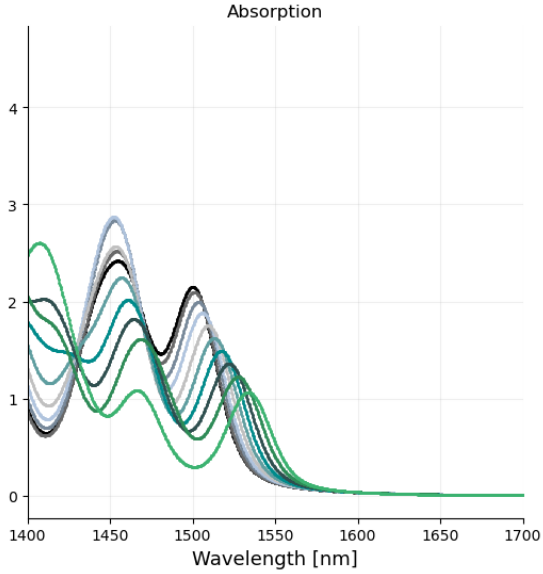
layer3 = Layer(InGaAlAs_material(1000.00), 30)

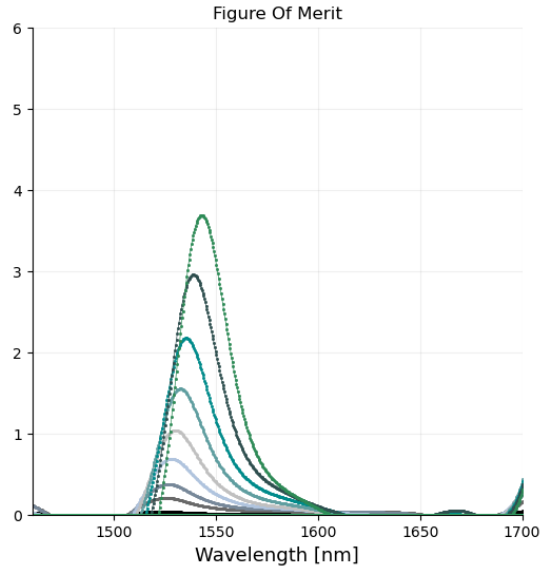
layer4 = Layer(InGaAlAs_material(1650.85), 30)

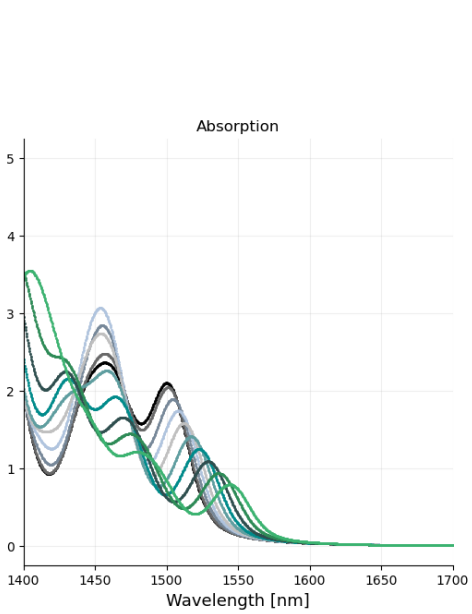
layers = [InP_layer2,layer3, layer4, layer2, layer1, InP_layer2]

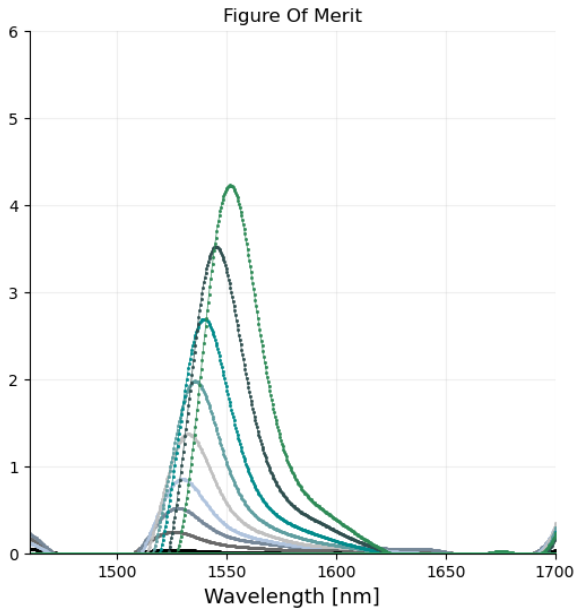



```
out: 1500.4150341586424
```









InP_layer2 = Layer(InGaAlAs_material(1239.85), 100)

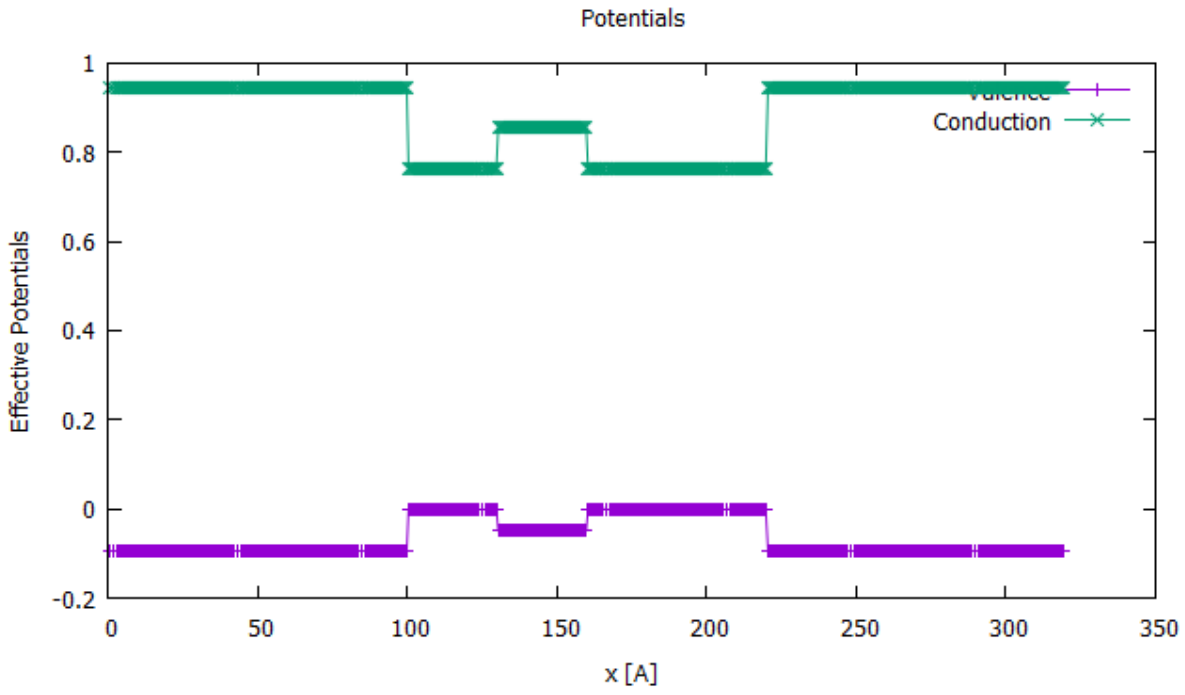
layer1 = Layer(InGaAlAs_material(1650.85), 60)

layer2 = Layer(InGaAlAs_material(1400.85), 30)

layer3 = Layer(InGaAlAs_material(1000.00), 30)

layer4 = Layer(InGaAlAs_material(1650.85), 30)

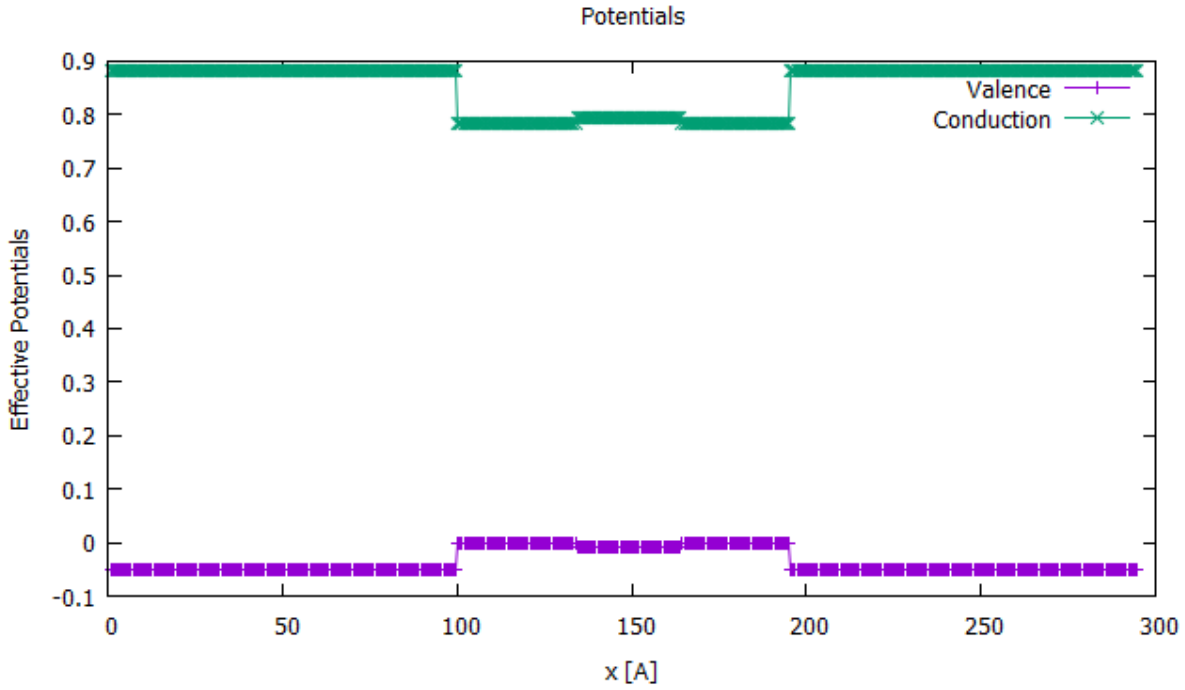
layers = [InP_layer2, layer4, layer2, layer1, InP_layer2]



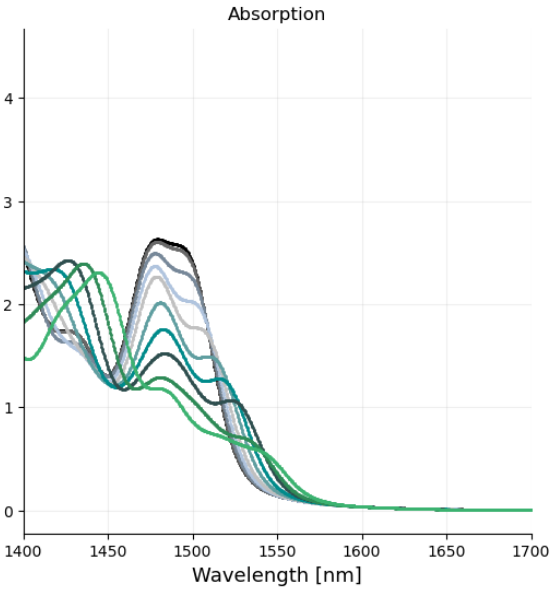
ML:

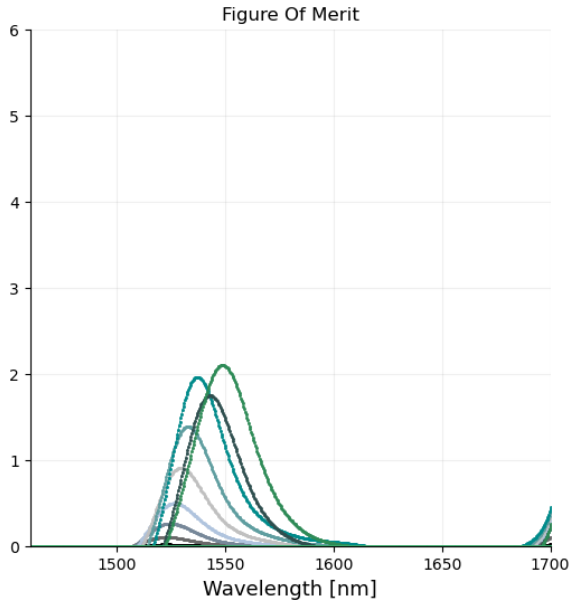
```
NeuralNetwork(
  (fc1): Linear(in_features=37, out_features=256, bias=True)
  (fc2): Linear(in_features=256, out_features=256, bias=True)
  (fc3): Linear(in_features=256, out_features=4, bias=True)
)


Had Mean Squared Error (MSE) on test data: 0.1822
```

Not good enough. Less is more in this case.



Optimized thicknesses: [33.8699494888415, 30.29662267776925, 31.023086845318318]
Optimized bandgaps: [1327.6670872844054, 1583.6467813671497, 1545.3039375807575, 1584.7255050729314]





Initial guess for thicknesses and bandgaps

initial_thicknesses = [30, 30, 60] # Example initial guess for thicknesses

initial_bandgaps = [1194.766898954708, 1624.720691840501, 1369.6999642066814, 1617.95942947708] # Example initial guess for bandgaps

```
Optimized thicknesses: [30, 30, 60]
Optimized bandgaps: [1194.766898954708, 1624.720691840501, 1369.6999642
066814, 1617.95942947708]
```

FAIL.. didn't generate any new designs.

Updated code so that penalties aren't just huge, but proportional to how far from 1500nm the generated design was:

New results:

InP_layer2 = Layer(InGaAlAs_material(1239.85), 100)

layer1 = Layer(InGaAlAs_material(1650.85), 60)

layer2 = Layer(InGaAlAs_material(1400.85), 30)

layer3 = Layer(InGaAlAs_material(1000.00), 30)

layer4 = Layer(InGaAlAs_material(1650.85), 30)

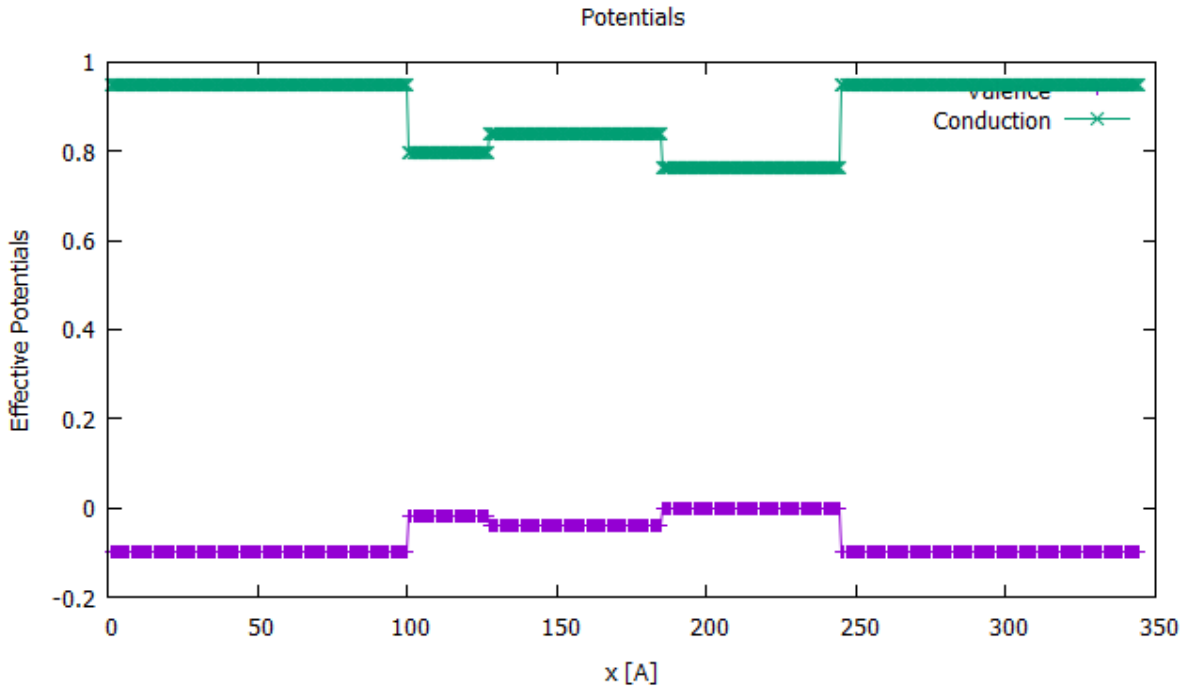
layers = [InP_layer2, layer4, layer2, layer1, InP_layer2]

initial_thicknesses = [30, 30, 60] # Example initial guess for thicknesses

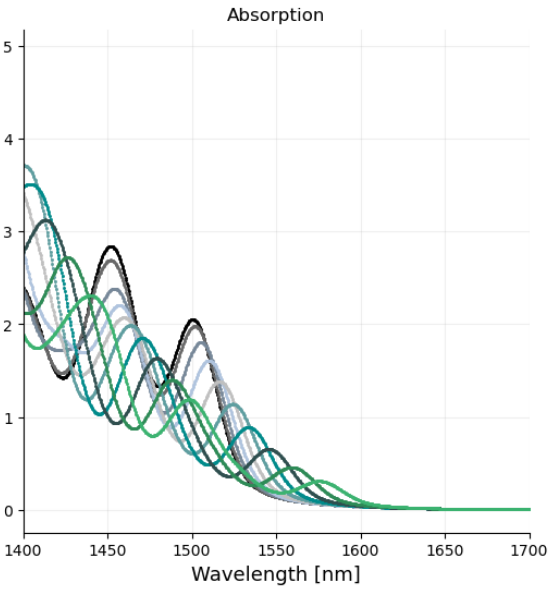
initial_bandgaps = [1194.766898954708, 1624.720691840501, 1369.6999642066814, 1617.95942947708] # Example initial guess for bandgaps

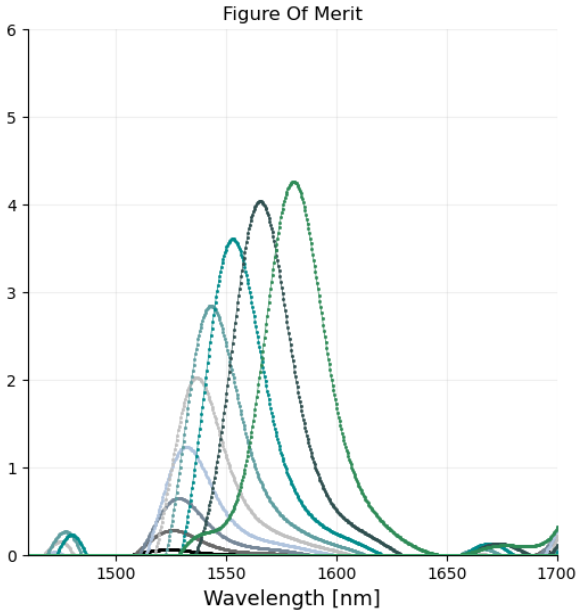
RESUKTS NEXT PAGE

Optimized thicknesses: [27.0, 58.15505279291747, 60.0]
Optimized bandgaps: [1184.3736555850817, 1523.37091950054, 1412.1710271
335708, 1625.1830535398785]



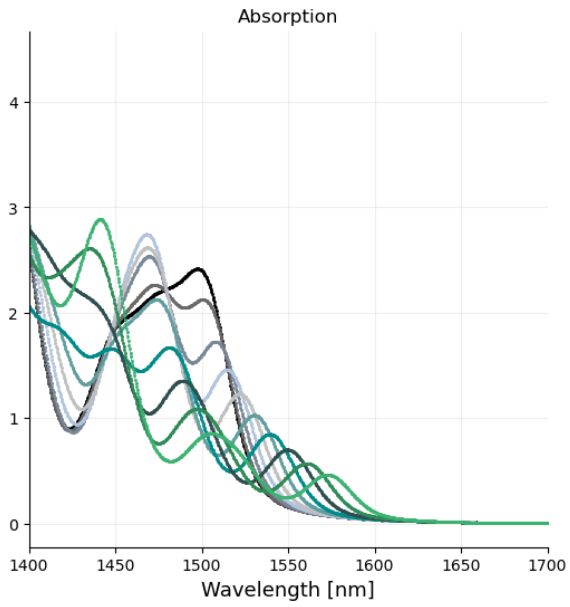
Very promising

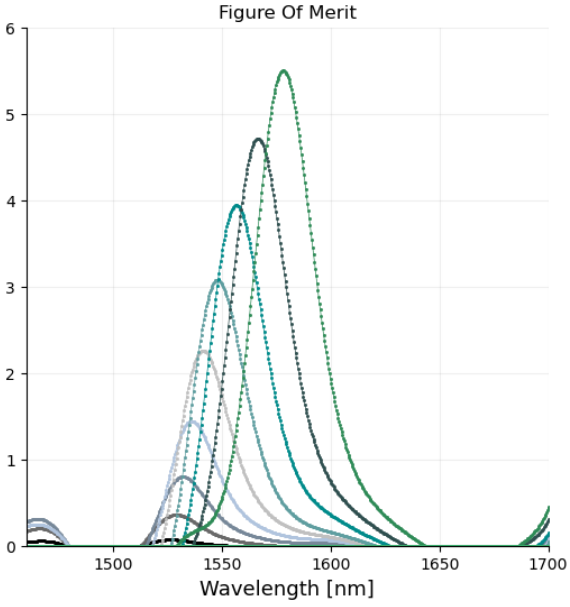


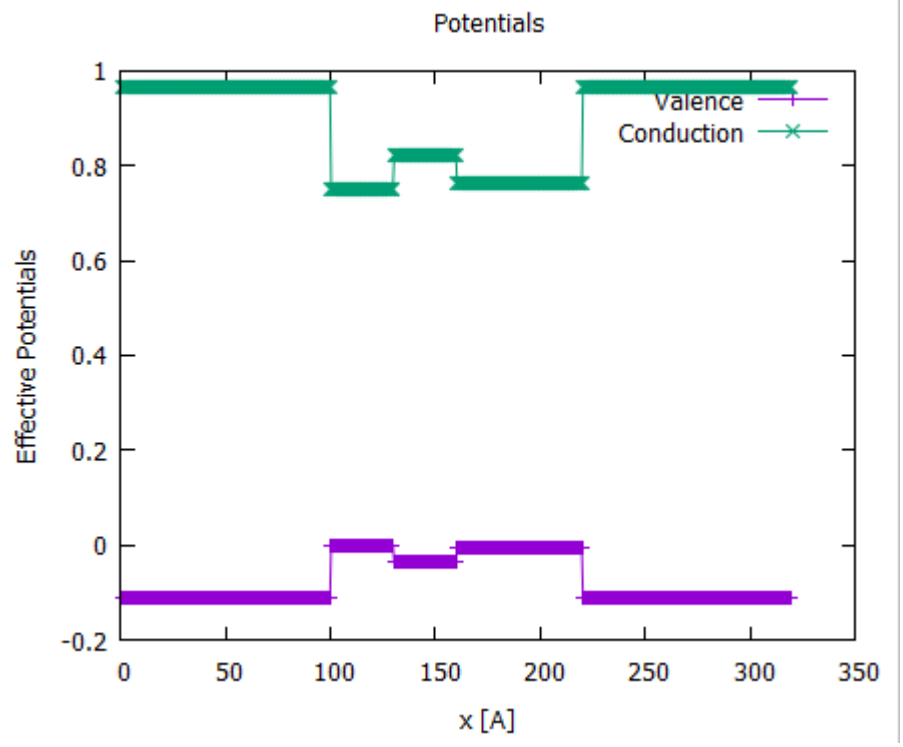


By making penalties to the optimisation algorithm less sever (simply the ab s difference of its bandgap from 1500nm), it converged on this:

```
# Initial guess for thicknesses and bandgaps
initial_thicknesses = [30, 30, 60]  # Example initial guess for thickne
sses
initial_bandgaps = [1194.766898954708, 1624.720691840501, 1369.69996420
66814, 1617.95942947708]  # Example initial guess for bandgaps

Optimized thicknesses: [30.0, 30.0, 60.0]
Optimized bandgaps: [1150.8489027773694, 1650.0, 1442.7959310371793, 16
05.7042835307416]
```

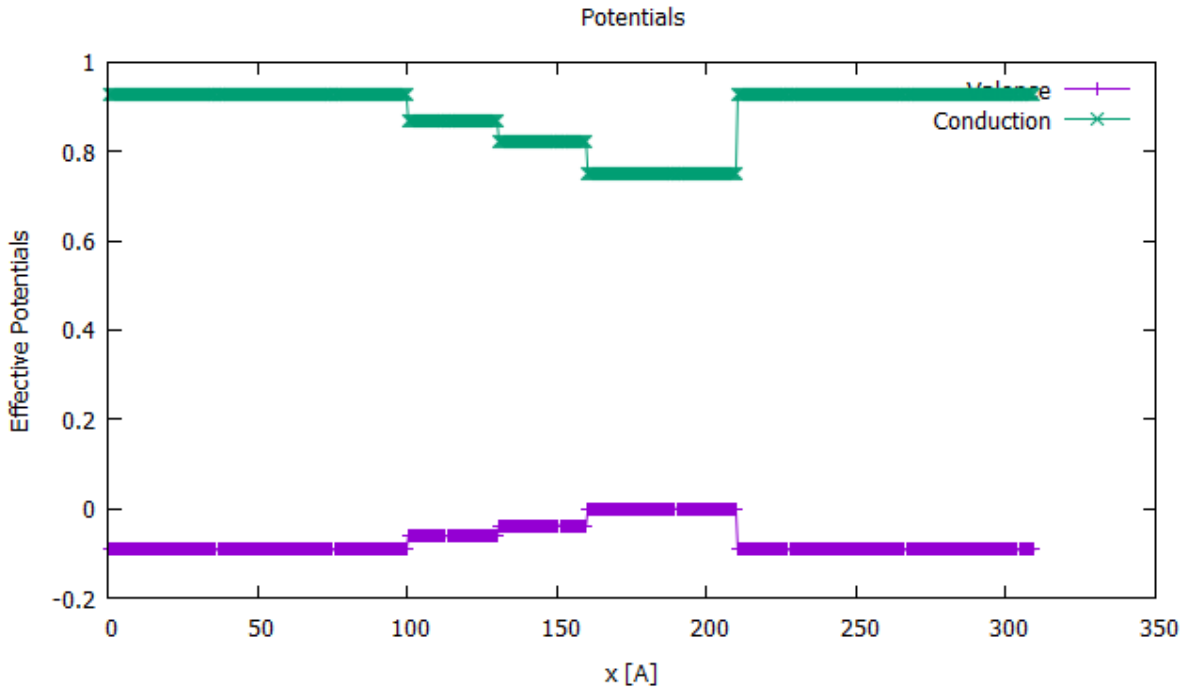






I think that this might be the full capability of the network. Further work required to fine tune and make it explore more possible solutions.

It's interesting to note that in observing the algorithm as it ran, thi s was not the last design it converged on. There were multiple points w here it was very obviously optimising other well variations. The last o bserved well looked like this:



And had a comparable FOM of 5+. It was actively trying to optimise this further, so I should maybe run the algorithm again for longer to see if it reconverges. These might have been the parameters it finished on:

```
Layers:
('In0.5274490000000001Ga0.199393Al0.273158As', 100.0)
('In0.528693Ga0.273341Al0.197966As', 51.56141154169549)
('In0.5297769999999999Ga0.337836Al0.132387As', 30.0)
('In0.5319422100000001Ga0.466521Al0.00153679As', 60.0)
('In0.5274490000000001Ga0.199393Al0.273158As', 100.0)
Materials:
GaAs: [0.111, 1.42, 0.063, 0.082, 0.51, 3.9476]
GaP: [-0.388, 2.74, 0.25, 0.14, 0.67, 3.3798]
InP: [0.0, 1.35, 0.077, 0.14, 0.6, 3.3688]
InAs: [0.441, 0.354, 0.023, 0.026, 0.41, 3.714]
AlAs: [-0.4245, 2.95, 0.15, 0.16, 0.79, 2.994]
In0.5274490000000001Ga0.199393Al0.273158As: [0.19306786108348928, 1.115
2432070849396, 0.065666786, 0.07376918, 0.53373934, 3.5140669378413545]
In0.528693Ga0.273341Al0.197966As: [0.23302281427323523, 0.9990613135410
433, 0.059075322, 0.06783454, 0.51256118, 3.5229108464492134]
In0.5297769999999999Ga0.337836Al0.132387As: [0.26455289586509545, 0.907
3774473245262, 0.053326588999999994, 0.062658674, 0.49409065999999996,
3.531805597770749]
In0.5319422100000001Ga0.466521Al0.00153679As: [0.3181540136457735, 0.75
15149356040317, 0.04185601233, 0.052331105860000005, 0.4572360802000000
6, 3.5427811664458315]
QWI Target Shift:
0.0
Number of Electric Fields:
10
```

Max Applied Electric Field:
10
FOM:
0
0
0
0

I have not yet looked how the trained network deals with QWI – I would expect that for a given heterostructure design the model should be able to know that the quality of the device decreases, and I'd expect that