Quantum Dot Design Technical Report

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Quantum Dot Problem

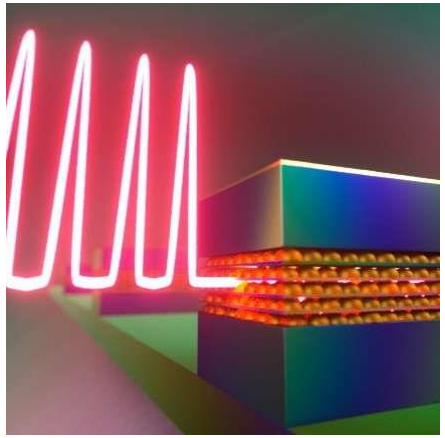
- High attention is given to Quantum Dots in the nanotechnology and material science worlds.
- Quantum Dots can select light wavelengths/energies and based on their design, absorbing and reflecting designed colors (frequencies) of light based on the specific physical and chemical parameters of their construction.
- Detailed throughout are the advantages, disadvantages, and design criteria that goes into designing a Quantum Dot.

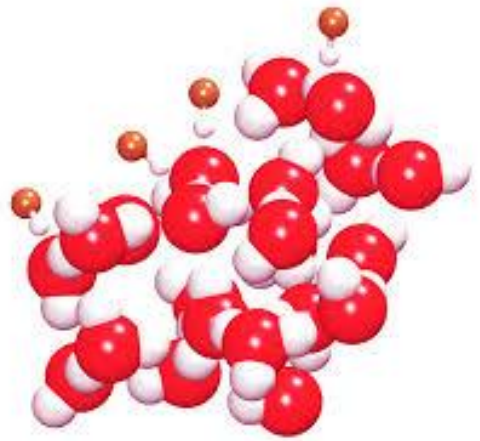
Why Care About Quantum Dots?

- **Absorber Uses**
  - »Detectors, Photodiodes, Solar Cells,
  - »Electromagnetic Shielding
- **Emitter Uses**
  - »TVs - QLEDs,
  - »Lasers / Optical Sources
  - »Transmission Systems
- **Atomic Modelling**
  - » Playground for Quantum Mechanics
  - » Atomic Chemistry -> Pharma, Biology, and Medical Applications
  - » Material Synthesis -> Battery Advancement

https://en.wikipedia.org/wiki/Solar_cell

https://phys.org/news/2018-03-quantum-dot-lasers-photonic-circuits.html





https://qcmm.udec.cl/

Solution Strategy Challenge 1

- This project will review the practical environmental and physical constraints which can be used as tunning devices for quantum dot energy absorption.
- These challenges represent the design approach one takes when designing a quantum dot.
- Versatility of quantum dots is revealed in this process as simulations uncover the wide breadth of results which various designs of quantum dots can have.
- These widely adaptable and manipulable quantum dots can be utilized in a wide range of applications, as each application requires a specific design.

Simple Quantum Dot Design (Quad Chart 1 of 2)

Objective:

- Design an intra-band absorber that absorbs A1=320±2meV with x polarized light and A2=470±2meV with y polarized light when illuminated from the top.

Problem:

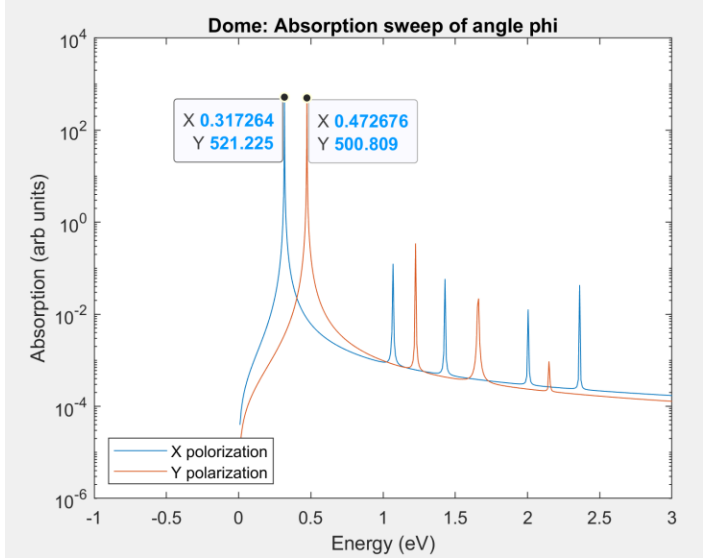
- Selecting the ideal structure.

Results / Impact:

- The absorption at the off-target energies are minimized in dome and cylinder compared to Pyramid.
- Pyramid and Dome's X, Y, Z dimensions were more interconnected than Cylinder's
- Dimensions were inversely proportional to Energy band across all structures

Approach:

- Performing simulations in the Quantum Dot Lab varying the structures and evaluate differences in simulation.
- Noting the control factors of each structure to use in solution refinement.



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Simple Quantum Dot Design (Quad Chart 2 of 2)

Objective:

- Design an intra-band absorber that absorbs A1=320±2meV with x polarized light and A2=470±2meV with y polarized light when illuminated from the top.

Problem:

- Honing into the specific energies

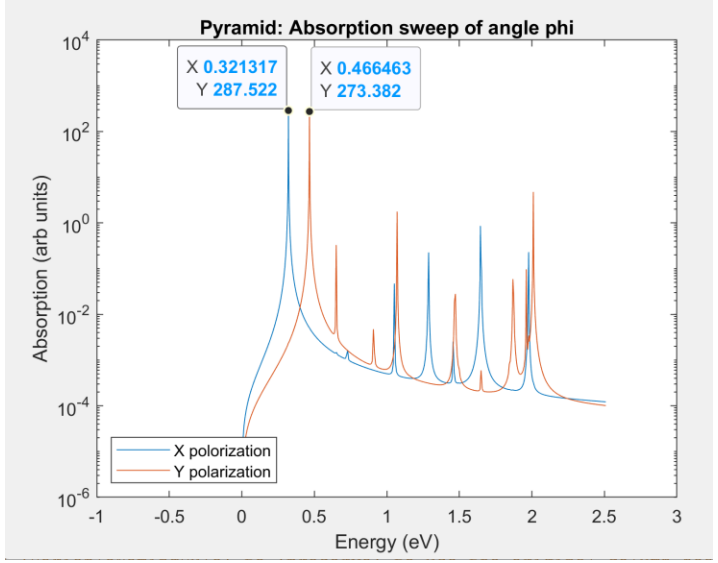
Approach:

- Quantum dot can be tuned to absorb specific energies.
  - Levers: X, Y, Z dimensions, m*
- Parameters were varied until ideal solution was found.

Results / Impact:

- Primary peaks at 321.3meV (x polarized) and 466.6meV (y polarized)
  - Note: absorptions >275
- Secondary peaks at 1.65eV (x polarized) and 2.01eV (y polarized)
  - Note: absorptions <5

x = 18.853nm
y = 14.481nm
z = 7.272nm
Lattice constant = 0.5nm
Effective mass = 0.04
Energy Gap = 0.7eV



Impact of Lattice Constant on Quantum Dot

Objective:

- Find how results depend on the lattice constant set

Problem:

- Lattice constant will change based on experiment conditions, such as temperature. How will this impact quantum dot characteristics?

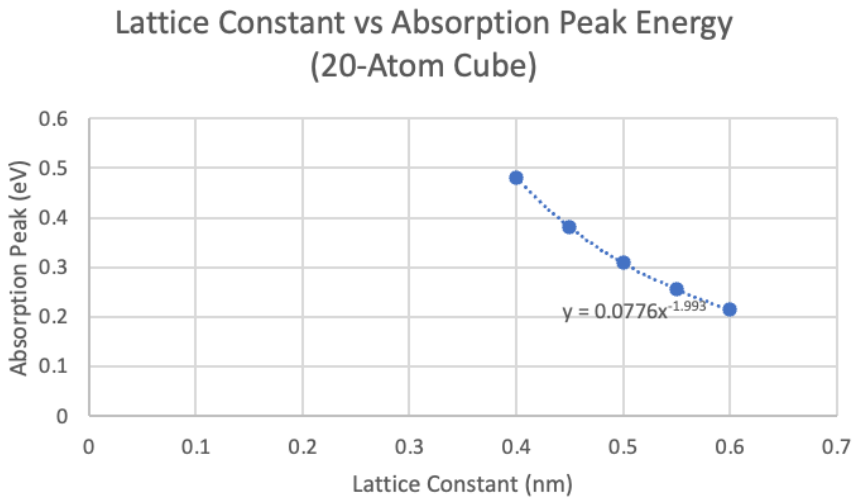
Results / Impact:

- Increasing lattice constant / atomic separation --> decreases spatial resolution, increases granularity
- Increasing lattice constant --> decreases Bandgap and location of absorption peaks

Approach:

- Increasing lattice constant increases physical dimensions of the Quantum Dot unit cell, decreases wavefunction overlap
- Discretized Schrödinger Equation: Energy inversely proportional to lattice constant "a"

$$E\psi_j = (U + \frac{\hbar}{ma})\psi_j - \frac{\hbar}{2ma}\psi_{j+1} - \frac{\hbar}{2ma}\psi_{j-1}$$



Variations in Quantum Dot Size

Objective:

- How stable is the solution against size variations of the physical structure.

Problem:

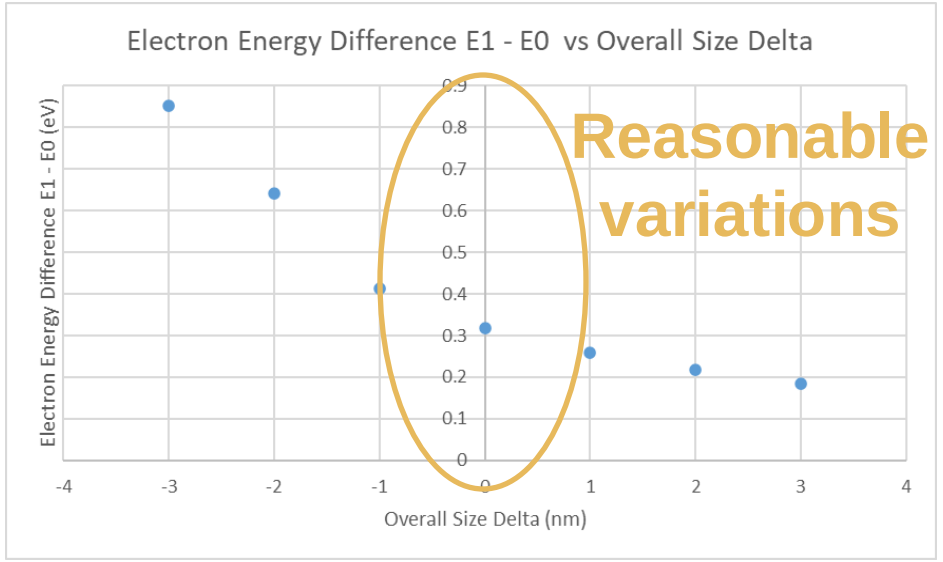
- Quantum dots characteristics are impacted by physical dimensions.

Results / Impact:

- The bandgap is tunable by size
- Larger Quantum Dot --> Smaller Bandgap, Absorption peaks at smaller energies
- Size of Quantum dot inversely proportional to transition energies

Approach:

- Reasonable variation experimentally due to annealing temperature (+-1nm) [3]
- Vary overall x, y, z size of quantum dot solution far greater and less than 1nm to find overall relationship



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Excited States of a Perfect Cube

Objective:

- Understand the excited states of a 10x10x10nm^3 cube

Problem:

- The excited states present unideal excited state wavefunctions.

Results / Impact:

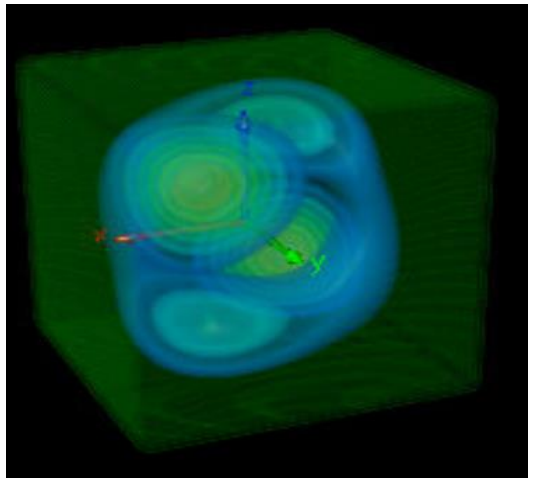
- Electron ground state energy = 1.011eV, first excited state energy = 1.320eV
- Perfect Cuboid: Some states will have same Energy values but different wavefunctions
- Simulation is accurate, and results in "Messier" Wavefunctions at higher energy orbitals

Approach:

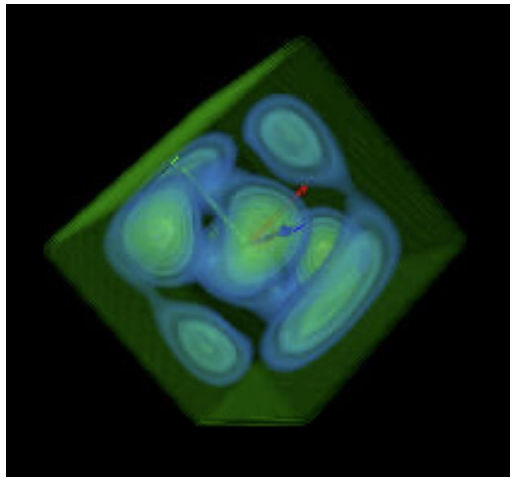
- With m* = .04 and Eg = .7eV simulate 10x10x10 cuboid
- Cuboid, compared to other more realistic structures, the wavefunction and energy is:

$$\psi(x,y,z) = \mathrm{A}\sin\left(\frac{\mathrm{n_x}\pi\mathrm{x}}{\mathrm{L}}\right)\sin\left(\frac{\mathrm{n_y}\pi\mathrm{y}}{\mathrm{L}}\right)\sin\left(\frac{\mathrm{n_z}\pi\mathrm{z}}{\mathrm{L}}\right)$$

$$E_{xyz} = \frac{\pi^2\hbar^2}{2m^*L^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$



Energy Level #7 1.629eV



Energy Level #14 2.1342eV

Variations in Fermi Level or Temperature (Quad Chart 1 of 2)

Objective:

- Understand the relationship between Fermi level and temperature to energy.

Problem:

- How does the Fermi level or temperature alter the design?

Results / Impact: Temperature

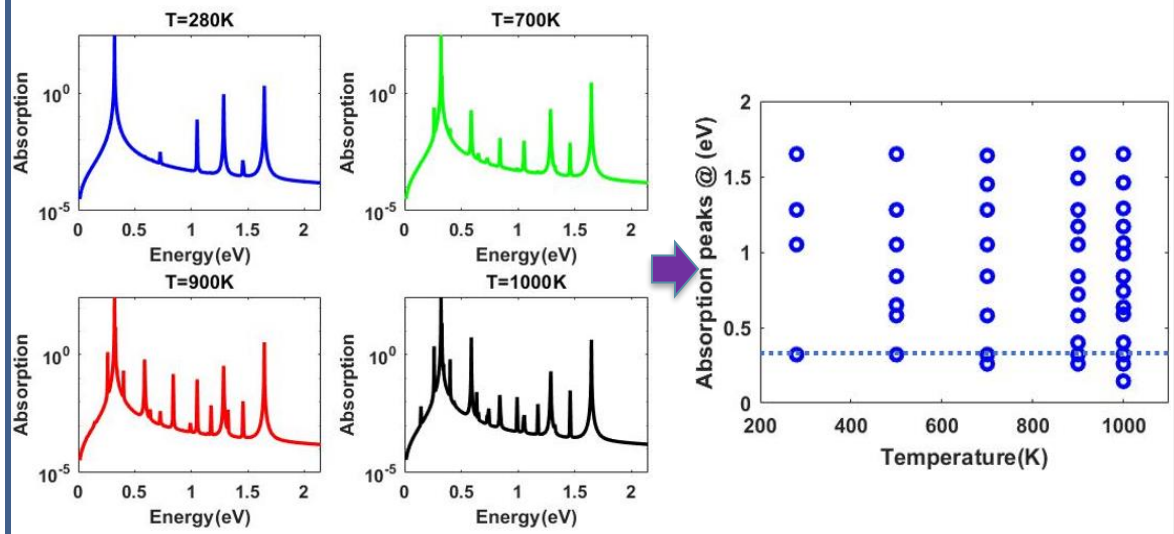
- Fermi level and Temperature both display most prominently in the **occupation of states** and intrinsic carrier count
- With an increase in Temperature beyond 300K, significant off-target peaks shows up ⟹ more noise in Quantum dot
- Absorption strength doesn't vary much

Approach:

- Vary the two parameters in simulation
- Compare with the literature on Density-Of-States and state occupation

$$n_i \propto \int_{E_c}^{\infty} f(E) * D(E)$$

$$n(E) \propto (1 + e^{\frac{E - E_f}{k_b T}})^{-1} * D(E)$$



Variations in Fermi Level or Temperature (Quad Chart 2 of 2)

Objective:

- Understand the relationship between Fermi level and temperature to energy.

Problem:

- How does the Fermi level or temperature alter the design?

Results / Impact: Fermi Level

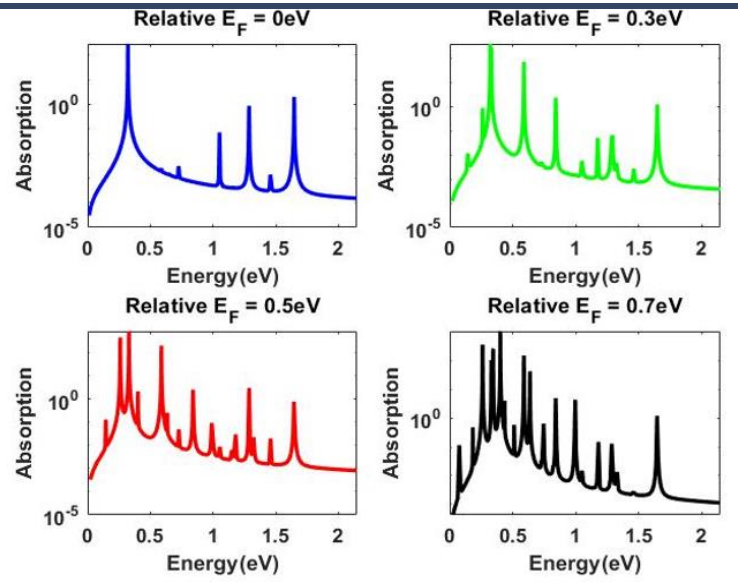
- Similar effect in terms of increased noise with increasing Fermi Energy, Ef (relative to Conduction Band energy)
- Absorption strength is also increased

Approach:

- Vary the two parameters in simulation
- Compare with the literature on Density-Of-States and state occupation

$$n_i \propto \int_{E_c}^{\infty} f(E) * D(E)$$

$$n(E) \propto (1 + e^{\frac{E - E_f}{k_b T}})^{-1} * D(E)$$



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Absorption Spectra on High Energies

Objective:

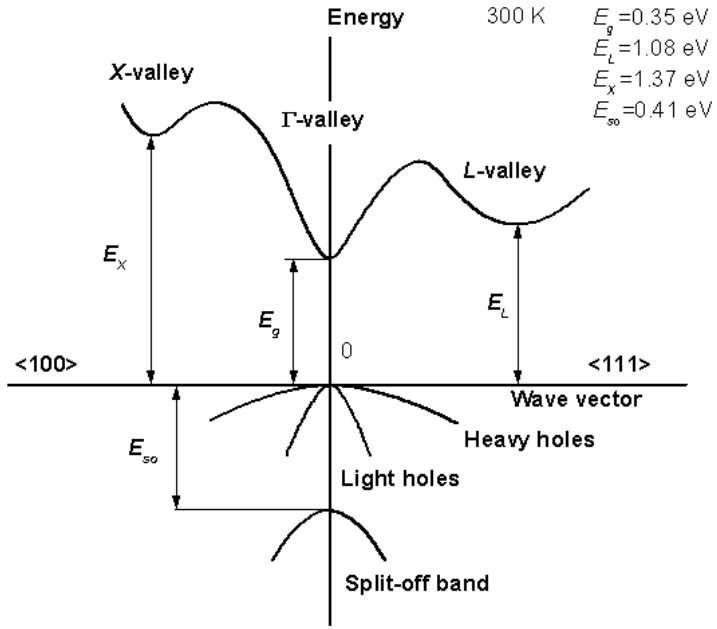
- Convey the validity of the absorption spectra for high energies

Approach:

- A Numeric Evaluation of the E-k dispersion of Indium Arsenide reveals its direct bandgap nature
- Any energies above E_g(=350meV) will be candidates for valence-to-conduction transitions in addition to intra-conduction-band excitations

Results / Impact:

- At higher energies, direct/band-to-band photogeneration is observed beyond simple excitation
- The simple quantum dot simulations used do not account for this behavior



https://www.ioffe.ru/SVA/NSM/Semicond/InAs/bandstr.html

Simulation Limitations (Quad Chart 1 of 2)

Objective:

- Reflect on the limitations of the simulations performed based on research papers.

Problem:

- Nanohub Quantum Dot Lab is a simulation tool which varies from real world experimentation.

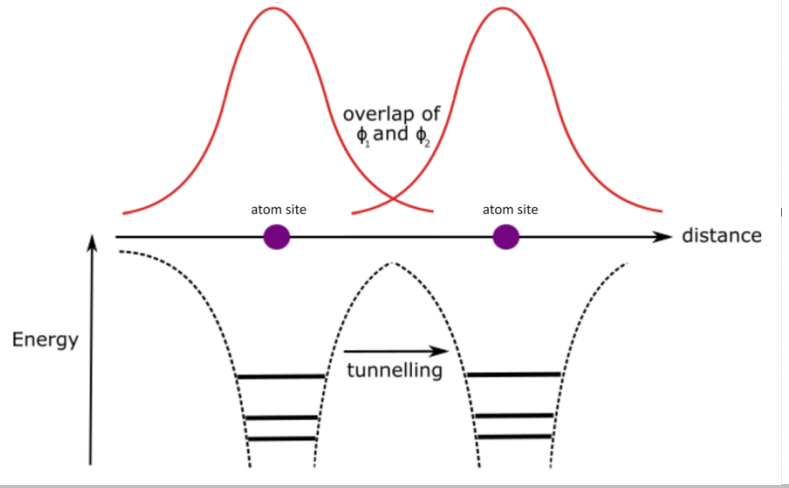
Results / Impact:

- TBM assumes the structure, and little overlap of atomic orbitals[4]
- TBM does not allow for total relaxation, where bonds can change
- TBM less accurate when number of neighbors is large [5]

Approach:

- Nanohub Quantum dot & modeling lectures for background knowledge
- NEMO 3-D uses Hamiltonian tight binding model (TBM) [8]

Tight Bandgap Model[9]



Simulation Limitations (Quad Chart 2 of 2)

Objective:

- Reflect on the limitations of the simulations performed based on research papers.

Problem:

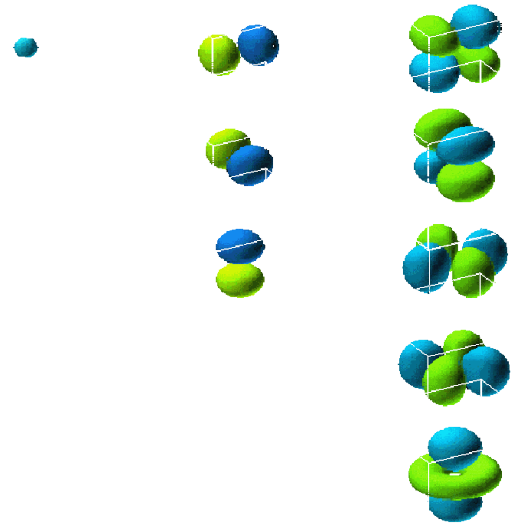
- Nanohub Quantum Dot Lab is a simulation tool which varies from real world experimentation.

Results / Impact:

- TBM valid for tens of thousands to tens of millions of atoms or less[7]
- Does not consider nonuniform atomistic composition[6]
- Strain limited to 8%[8]

Approach:

- NEMO 3-D uses Hamiltonian tight biding model (TBM)[8]
- NEMO 3-D uses TBM to reproduce bulk band properties of semiconductors[8]
- Strain is calculated using an atomistic valence force field (VFF) model[7]



Multilayer Discovery (Quad Chart 1 of 2)

Objective:

- Exploring Multilayer GaAs-InAs-GaAs Quantum dots

Problem:

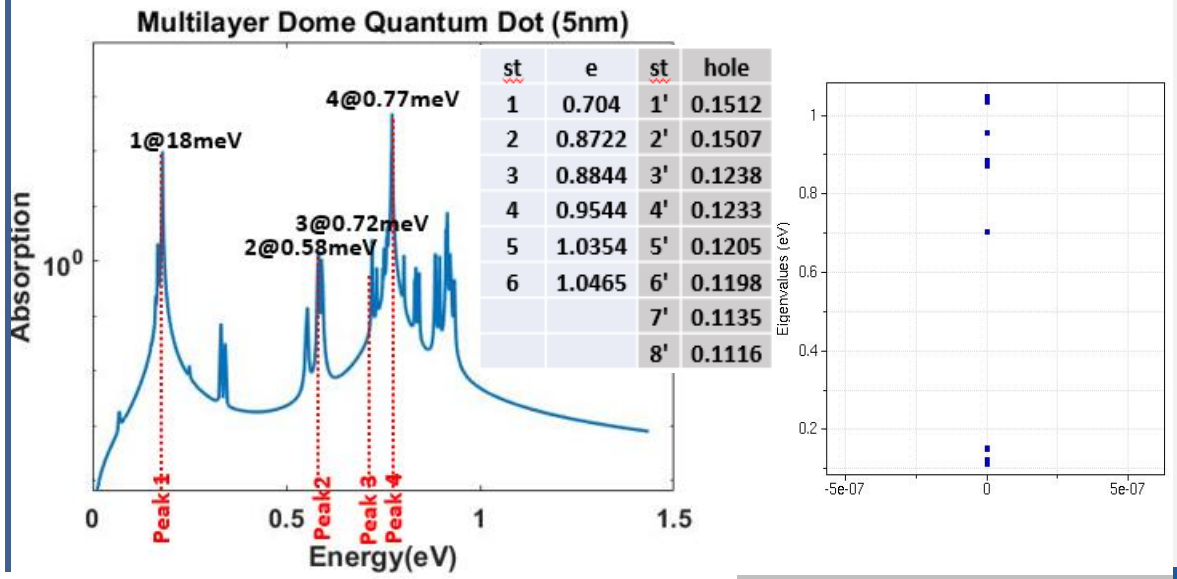
- Convergence issues in the simulator

Results / Impact:

- Band-to-band transitions dominate Absorption Spectra
- Peak1: Intraband transition from 1 to 3
- Peaks 2,3 and 4: Interband transition from 3' to1, from 1' to 2 and from 7' to 3
- Hole states are far more densely packed than electron states

Approach:

- Looking into the Electron and hole ground states and Absorption spectra to explain them in terms of Interband and Intraband transitions
- Exploring the effect of Substrate depth and Capping Layer by varying layer size



st	e	st	hole
1	0.704	1'	0.1512
2	0.8722	2'	0.1507
3	0.8844	3'	0.1238
4	0.9544	4'	0.1233
5	1.0354	5'	0.1205
6	1.0465	6'	0.1198
		7'	0.1135
		8'	0.1116

Multilayer Discovery (Quad Chart 2 of 2)

Objective:

- Exploring Multilayer GaAs-InAs-GaAs Quantum dots

Problem:

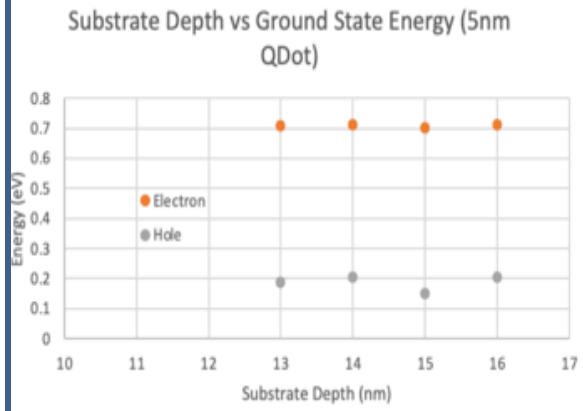
- Convergence issues in the simulator

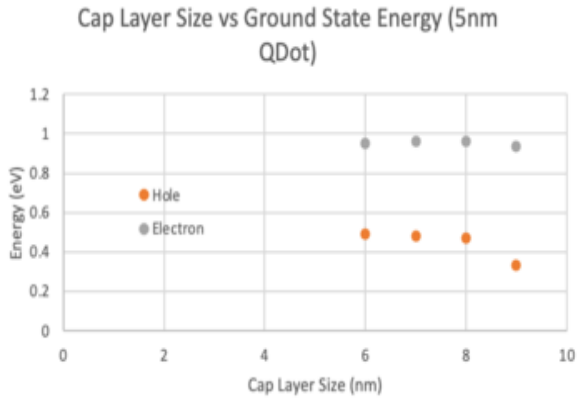
Results / Impact:

- As the structure is able to encapsulate more of the wavefunctions, the ground state energy decreases slightly.
- The hole wavefunction is broader, and therefore displays a more substantial impact when cap layer size is increased.

Approach:

- Looking into the Electron and hole ground states and Absorption spectra to explain them in terms of Interband and Intraband transitions
- Exploring the effect of Substrate depth and Capping Layer by varying layer size





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Multilayer Quantum Dot Design

Objective:

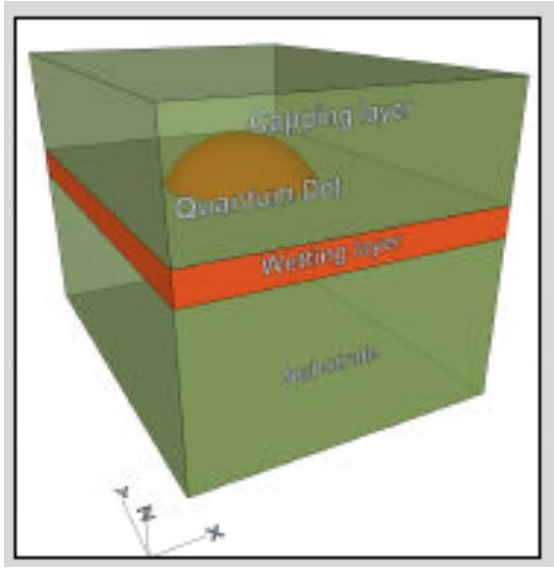
- Design an InAs quantum dot in GaAs that that absorbs A1=50meV±DE in the x direction and A2=100meV±DE in the y direction and minimizes in the z direction.

Results / Impact:

- Decreasing caping layer increases energy gap and location of absorption peaks
- Decreasing lateral domain size increases bandgap
- Decreasing substrate depth decreases bandgap
- Decreasing wetting layer decreases energy gap

Approach:

- "Two Band eff. Mass" used for first explorations of multilayered quantum dot
- Setting Fermi level just above electron ground state.
- Varying structure to observe different absorption band results



Multilayer Quantum Dot Design

Objective:

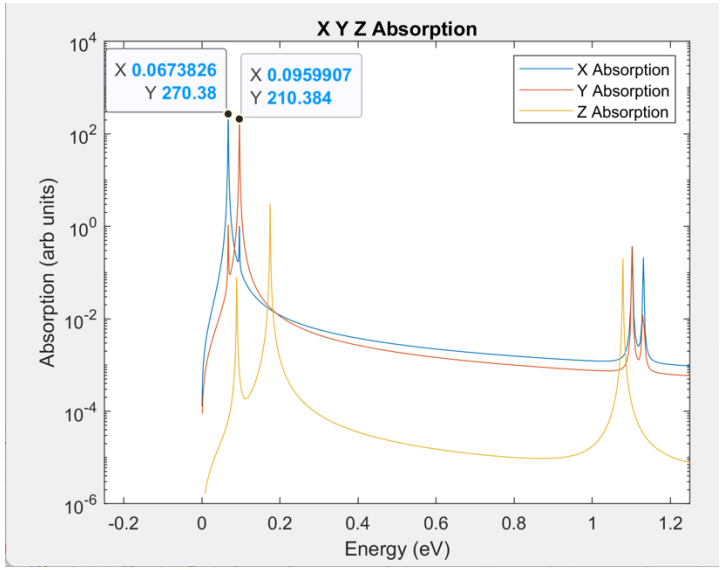
- Design an InAs quantum dot in GaAs that that absorbs A1=50meV±DE in the x direction and A2=100meV±DE in the y direction and minimizes in the z direction.

Results / Impact:

- Only consider cold temperatures 77K or below to reduce energy noise.
- Absorption in X direction: A1 = .06738eV
- Absorption in Y direction: A2 = .09599eV
- Absorption in Z direction magnitude minimized

Approach:

- Final simulation using material model “TB20 band 10 orb. sp3d5s_so” for strain
- Dome quantum dot used due to absorption peak shape
- Generally, higher X dimension and lower Z dimension results in lower energy absorption



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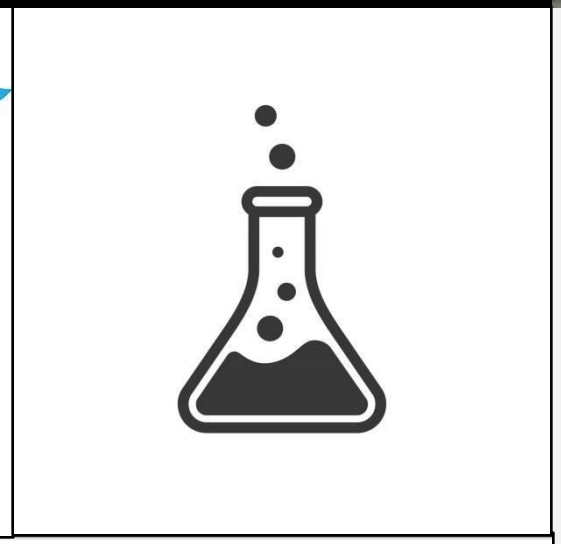
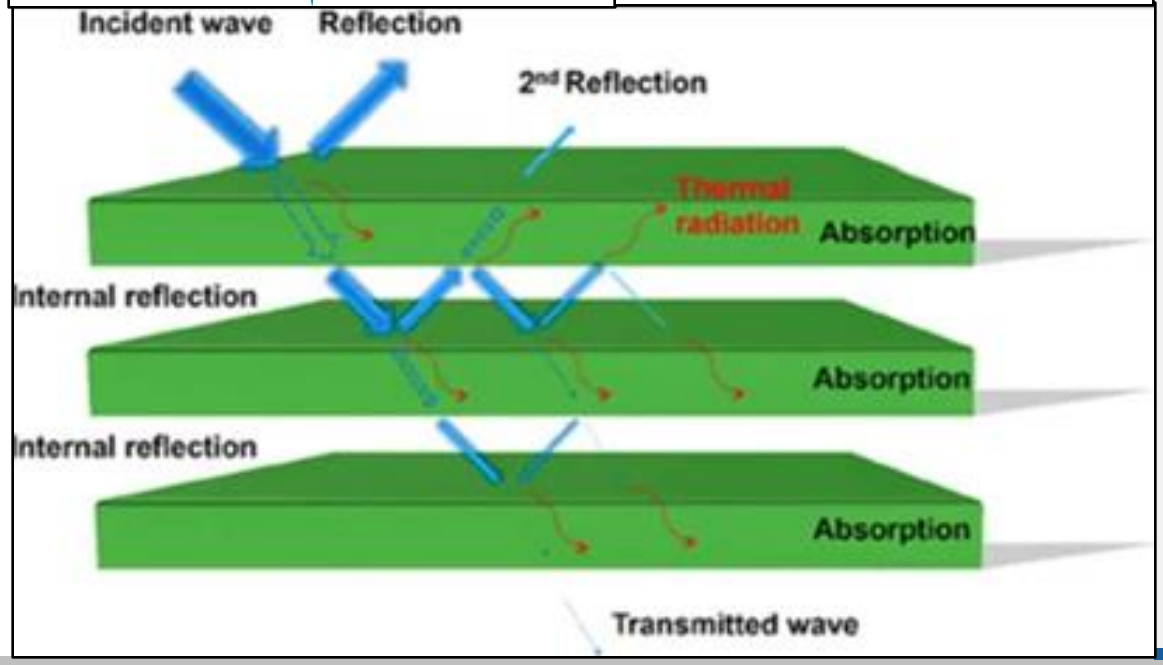
Reflection and Main Take Aways

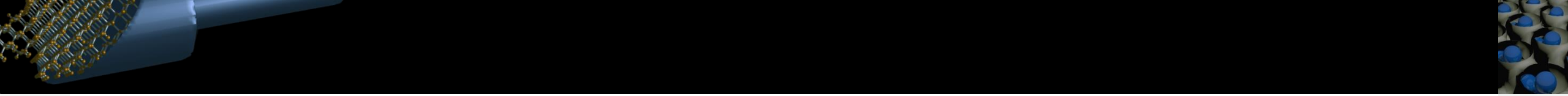
- Particle-in-a-box approximation
  - Well-conducting, low energy region surrounded by a poorly-conducting, high energy region in all three dimensions.
- Realistic Quantum Dots come in various structures
  - Dome, Pyramid, Cylinder, Spheroid, Cone
- Quantum Dots can be **tuned** to absorb **specific energies**
- Tuning Mechanisms
  - X, Y, Z Dimensions
  - Effective mass
  - Impurity concentrations
  - environment (multilayered)
- Quantum dots can be used to understand quantum mechanics and can be practically used for their ability to absorb and emit specific energies when tuned.

Going Forward...

- Quantum Dots are positioned to become increasingly **relevant**, **useful**, and **commonplace** in the next decade.
- They stand to help advance medicine, chemistry, technology, and make a greener planet.
- The knowledge gained in this project can be adapted to frequencies outside of the visible light spectrum. Aligning with emerging research this could aid in the creation of advanced EMI shielding.







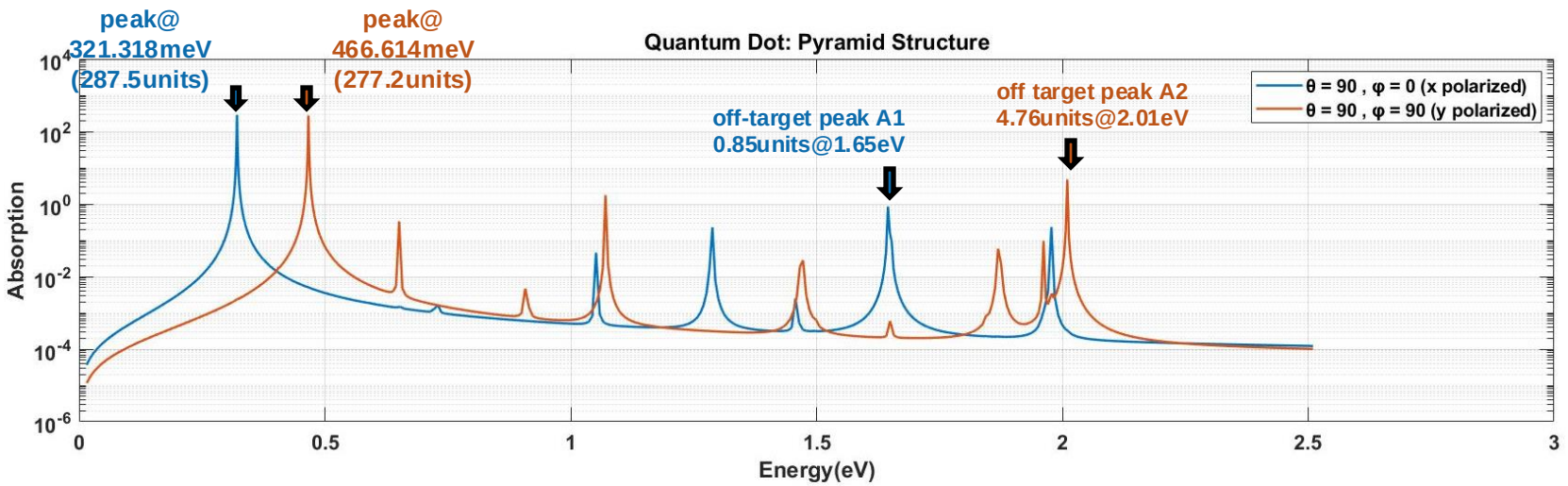
Appendices

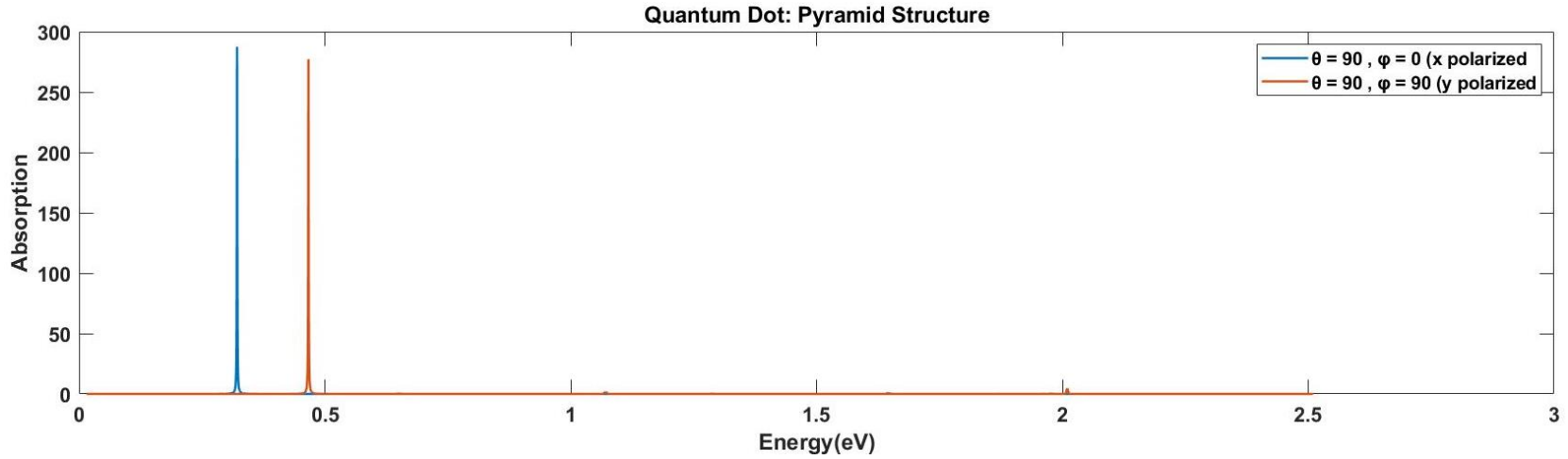
Team "Think Outside the Particle-in-a-Box"

- This team consisted of four members with distinct backgrounds split evenly between academic research and industry experience.
- The team effort focused on collaboration rather than a division of labor.
- To build a basis for this project, every member attempted Challenge 2 and collaborated on the final solution.
- All other challenges had at least two members, with members choosing challenges they were particularly interested in or had a background in. The team collaborated on the final solution.
- Utilized meetings to discuss final solutions and shared messing app to collaborate when "stuck" on a problem

Additional Detail on Challenge 1 Final Solution

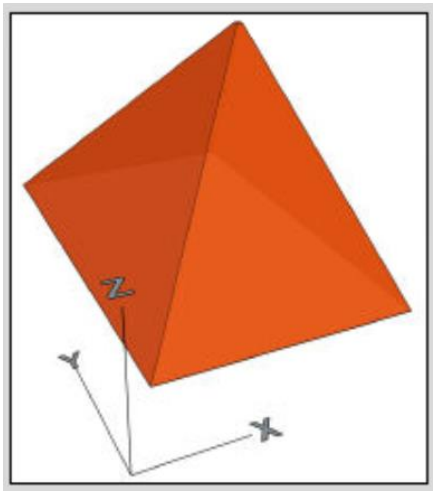
- Pyramid Quantum Dot Solution for Challenge 1:





Optimized Parameters for Quantum Dot: Pyramid

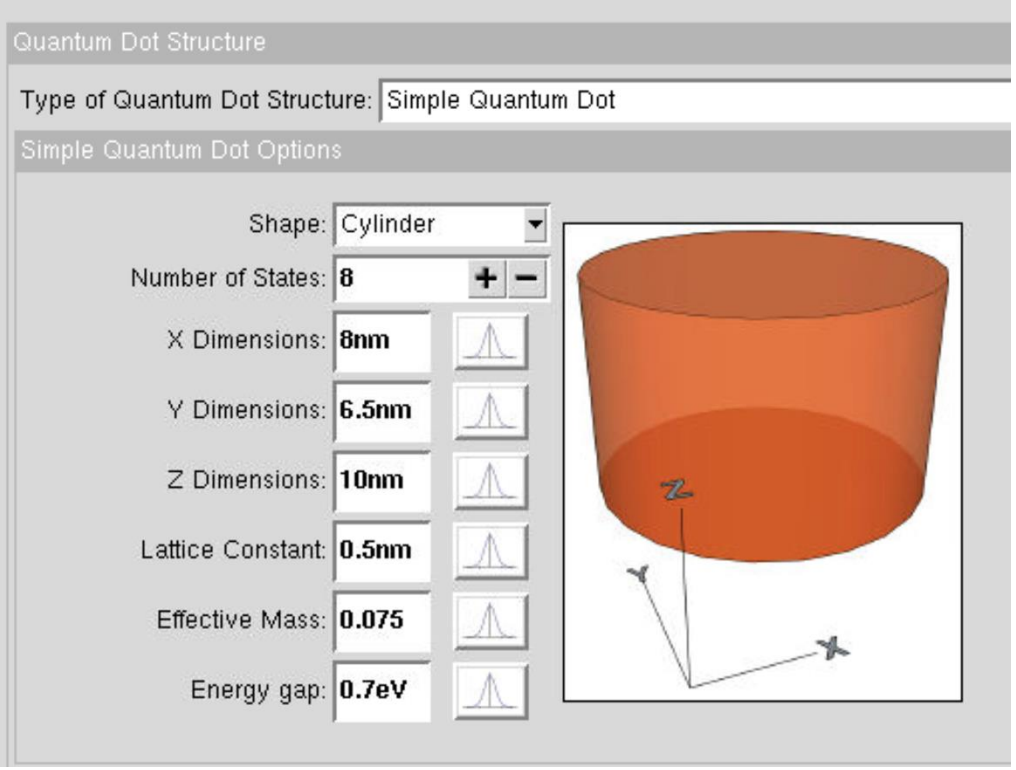
x = 18.853nm
y = 14.481nm
z = 7.272nm
Lattice constant = 0.5nm
Effective mass = 0.04
Energy Gap = 0.7eV



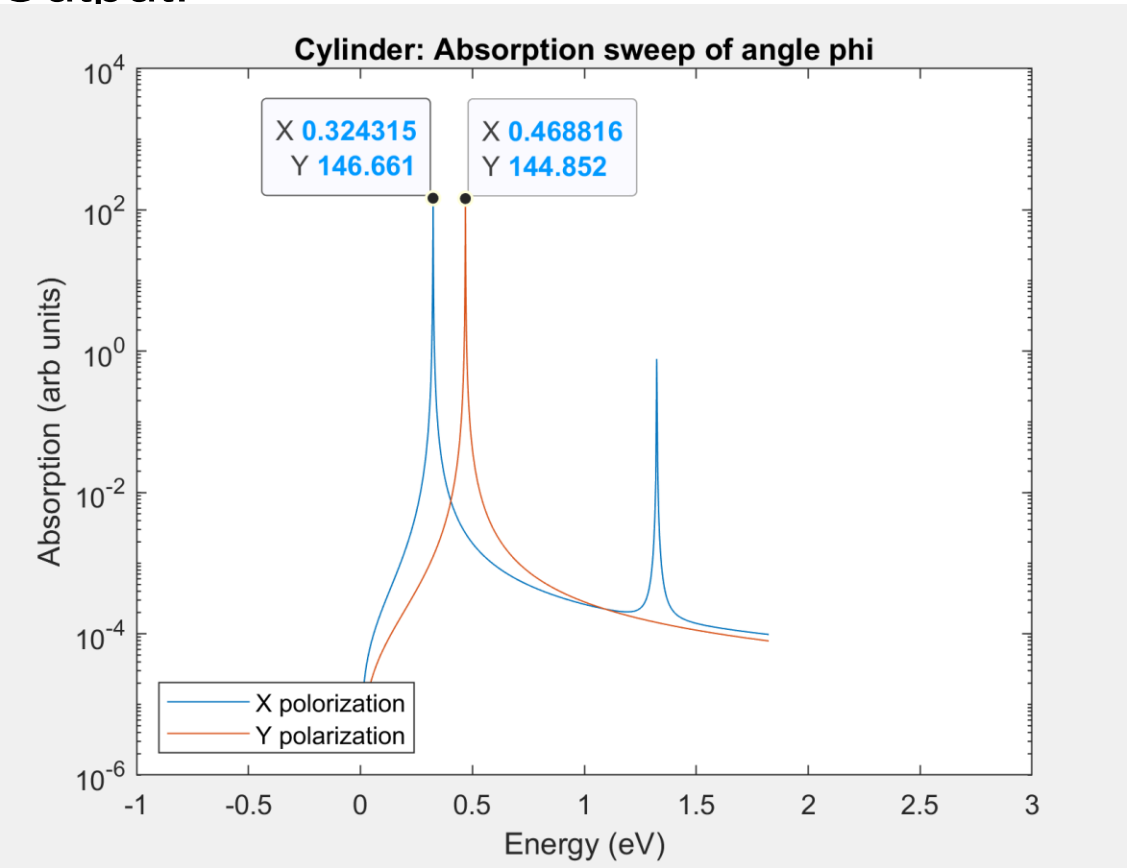
Additional Detail on Challenge 1 Final Solution

- Cylinder Quantum Dot Solution for Challenge 1:

Input Dimensions:



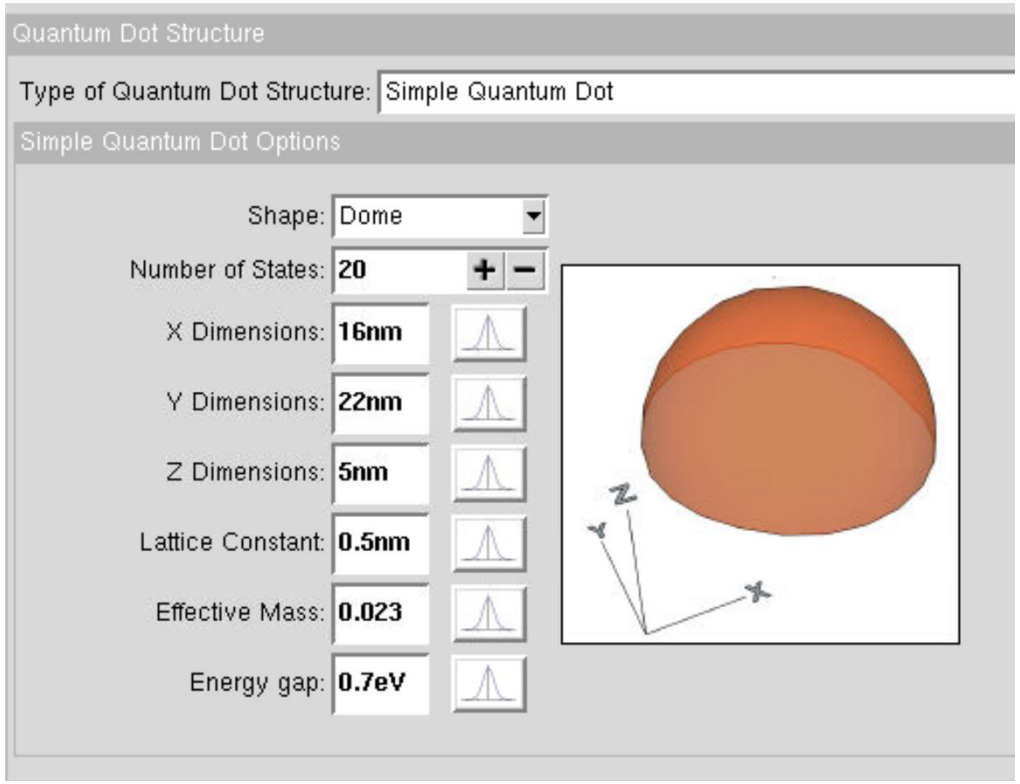
Output:



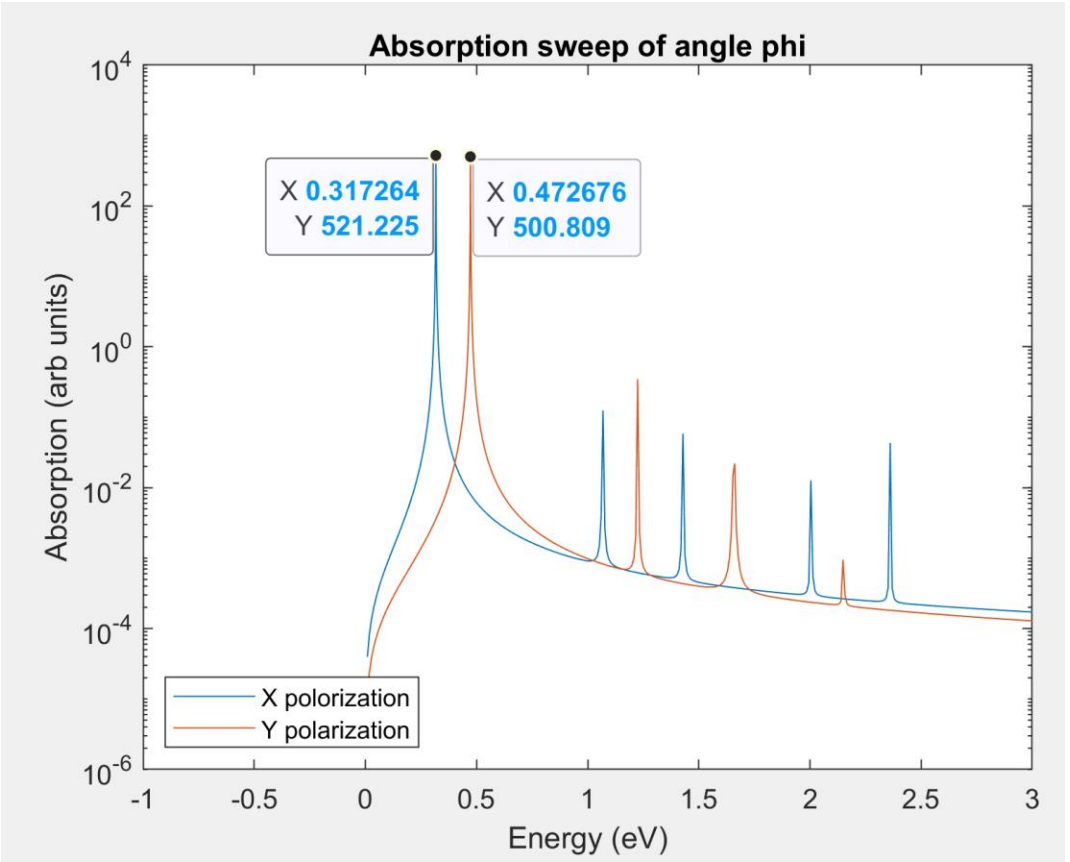
Additional Detail on Challenge 1 Final Solution

- Dome Quantum Dot Solution for Challenge 1:

Input Dimensions:



Output:



Additional Detail on Challenge 4

Wavefunctions do not look so clean for 10x10x10 nm^3 cuboid structure
because of degeneracy of energy states.

For a Cubic 3D Quantum dot, the wavefunction and the Eigen energy

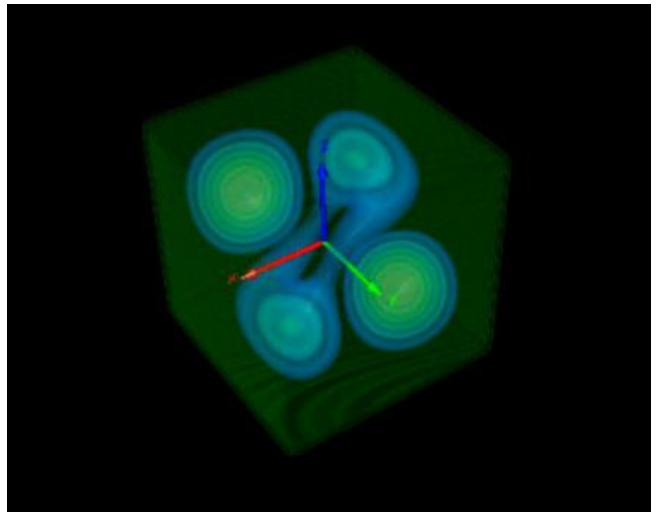
$$\psi(x,y,z) = \mathrm{A}\sin\left(\frac{\mathrm{n_x}\pi \mathrm{x}}{\mathrm{L}}\right)\sin\left(\frac{\mathrm{n_y}\pi \mathrm{y}}{\mathrm{L}}\right)\sin\left(\frac{\mathrm{n_z}\pi \mathrm{z}}{\mathrm{L}}\right)$$

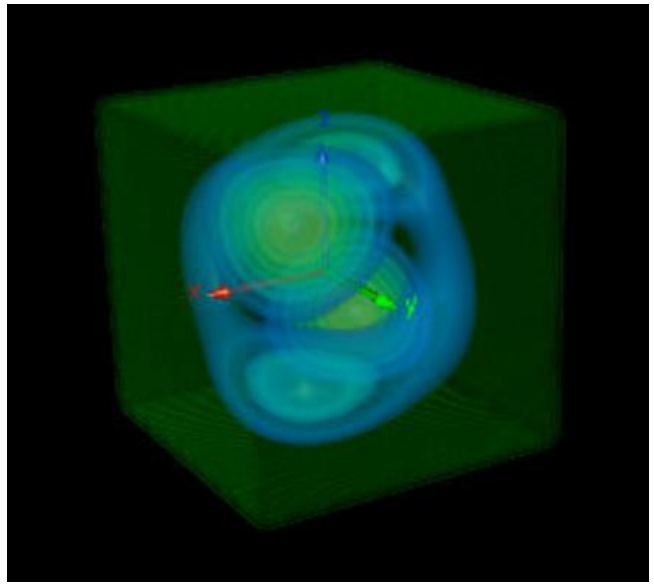
$$E_{xyz} = \frac{\pi^2\hbar^2}{2m^*L^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

For example, say (n_x, n_y, n_z) = (1,1,2) or (1,2,1) or (2,1,1)

These three states will have the same energy

But their wavefunctions are different, this is why the wavefunctions are not clean.





Particle-in-a-box Basis for Quantum Dot

- Quantum Dots can be approximated by particle-in-a-box because it is a well conducting low energy region, surrounded by a low conducting high energy region in all three dimensions.[2]

- Particle-in-a-box approximation[1]

$$\Delta E(r) = E_{\text{gap}} + \left(\frac{h^2}{8r^2}\right)\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right)$$

- Radius and effective mass of the dot is shown to be inversely proportional to energy gap. This holds true in the simple quantum dot simulation on nanohub.

Discretized Schrödinger Equation

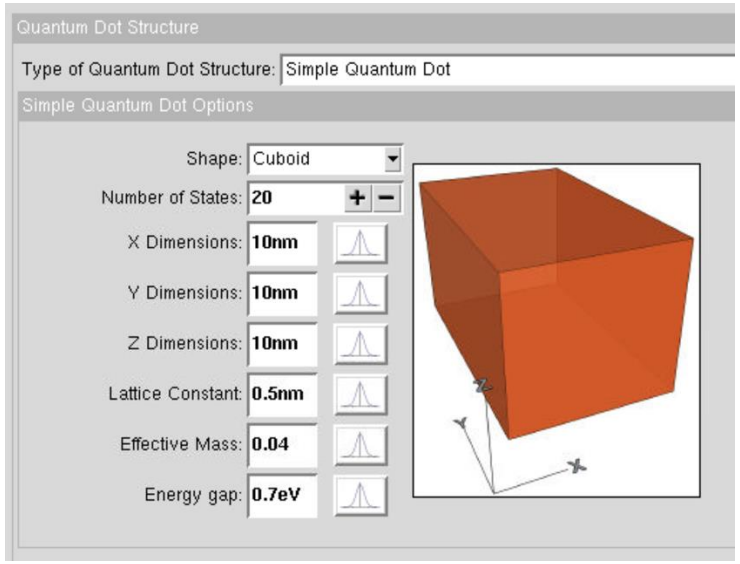
- From ECE606 Lecture 6.5

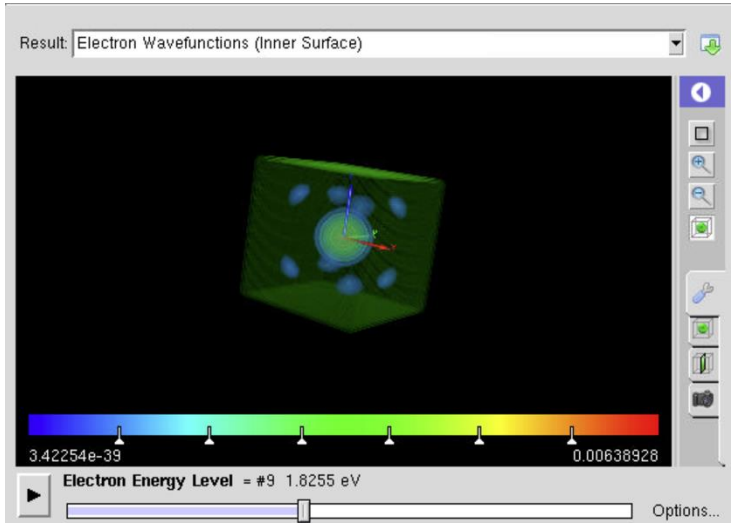
$$\boxed{-\left(t_0 a^2\right)\frac{d^2\psi}{dx^2}+U(x)\psi=E\psi} \qquad t_0 \equiv \frac{\hbar^2}{2m_0 a^2}$$

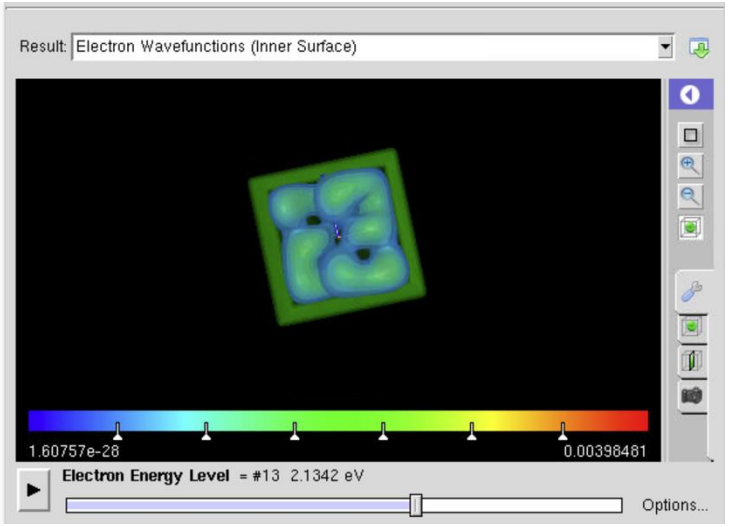
$$\mathbf{H}\psi = E\psi \qquad E\psi_j = (U+\frac{\hbar}{ma})\psi_j - \frac{\hbar}{2ma}\psi_{j+1} - \frac{\hbar}{2ma}\psi_{j-1}$$

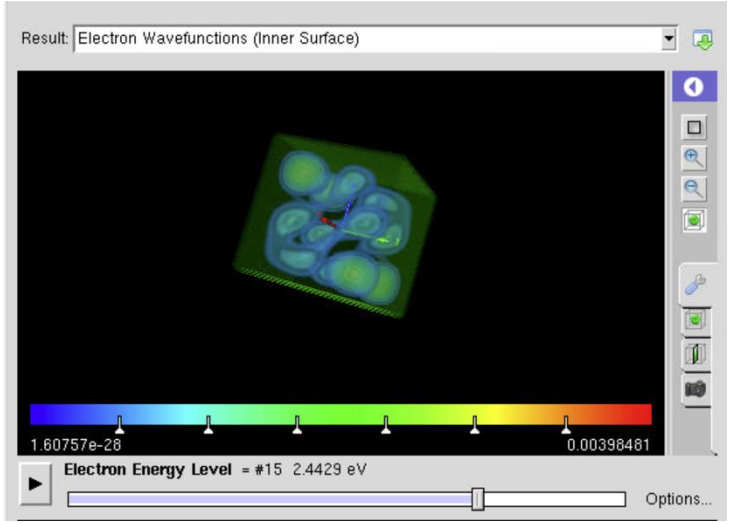
- Important relationships to observe from this derivation of discretized Schrodinger equation
  - Lattice constant "a" inversely proportional to Energy
  - Mass "m_0" inversely proportional to Energy

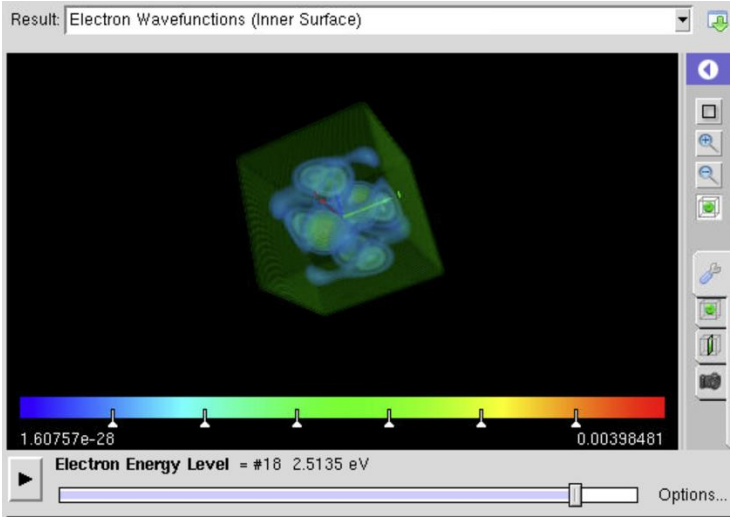
Excited States of Perfect Cube Example Wavefunctions



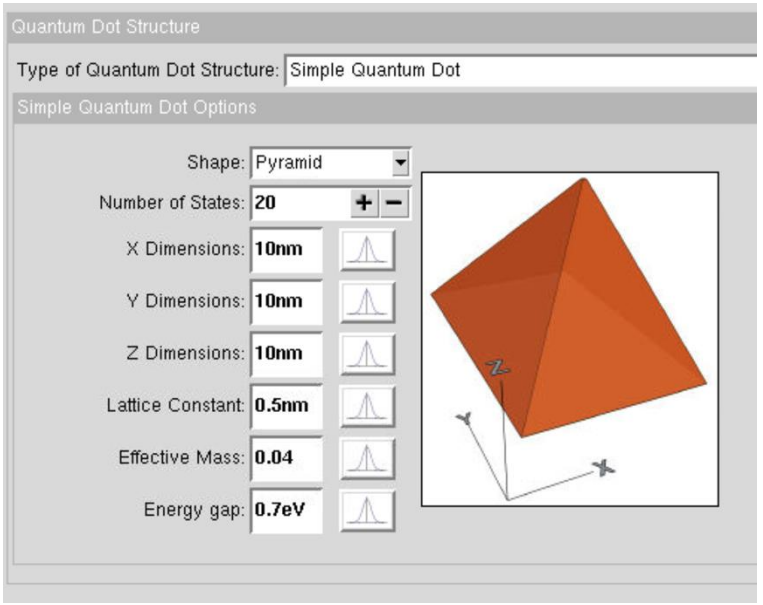


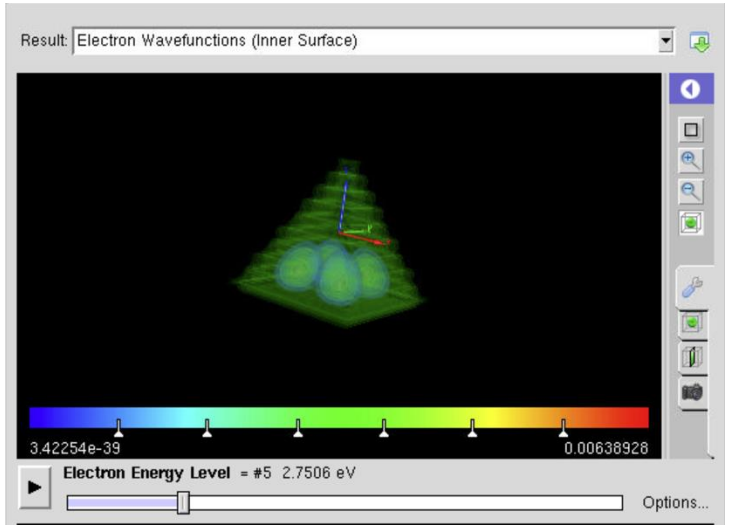


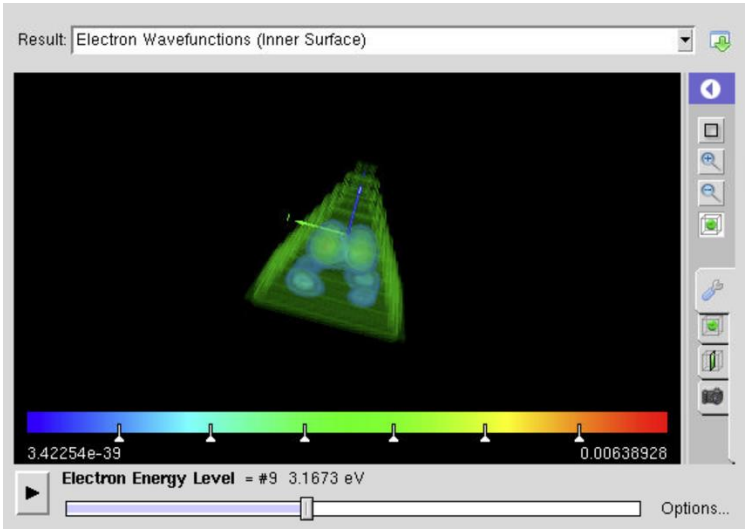


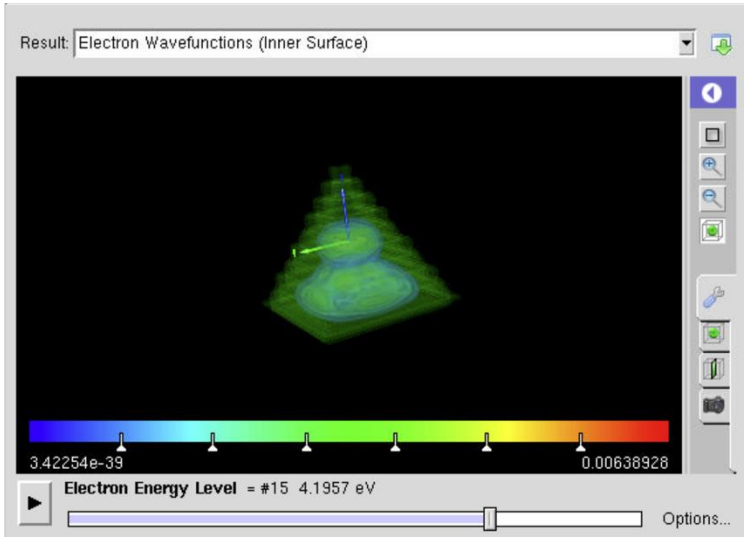


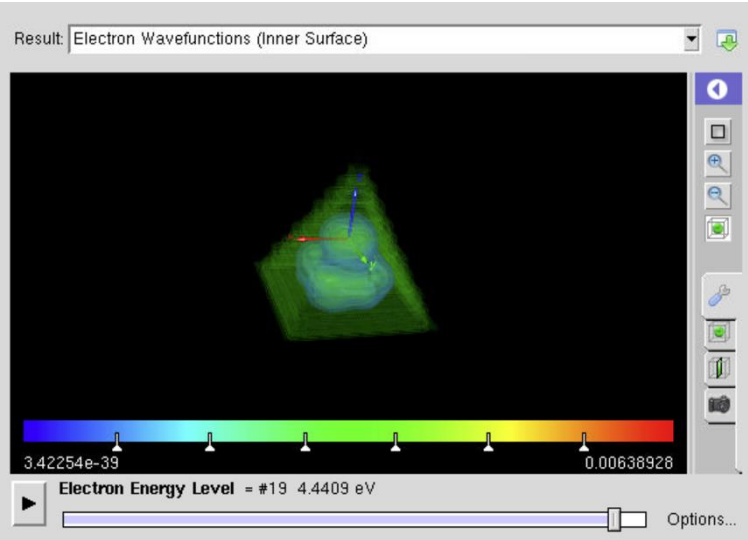
Excited States of Pyramid Example Wavefunctions











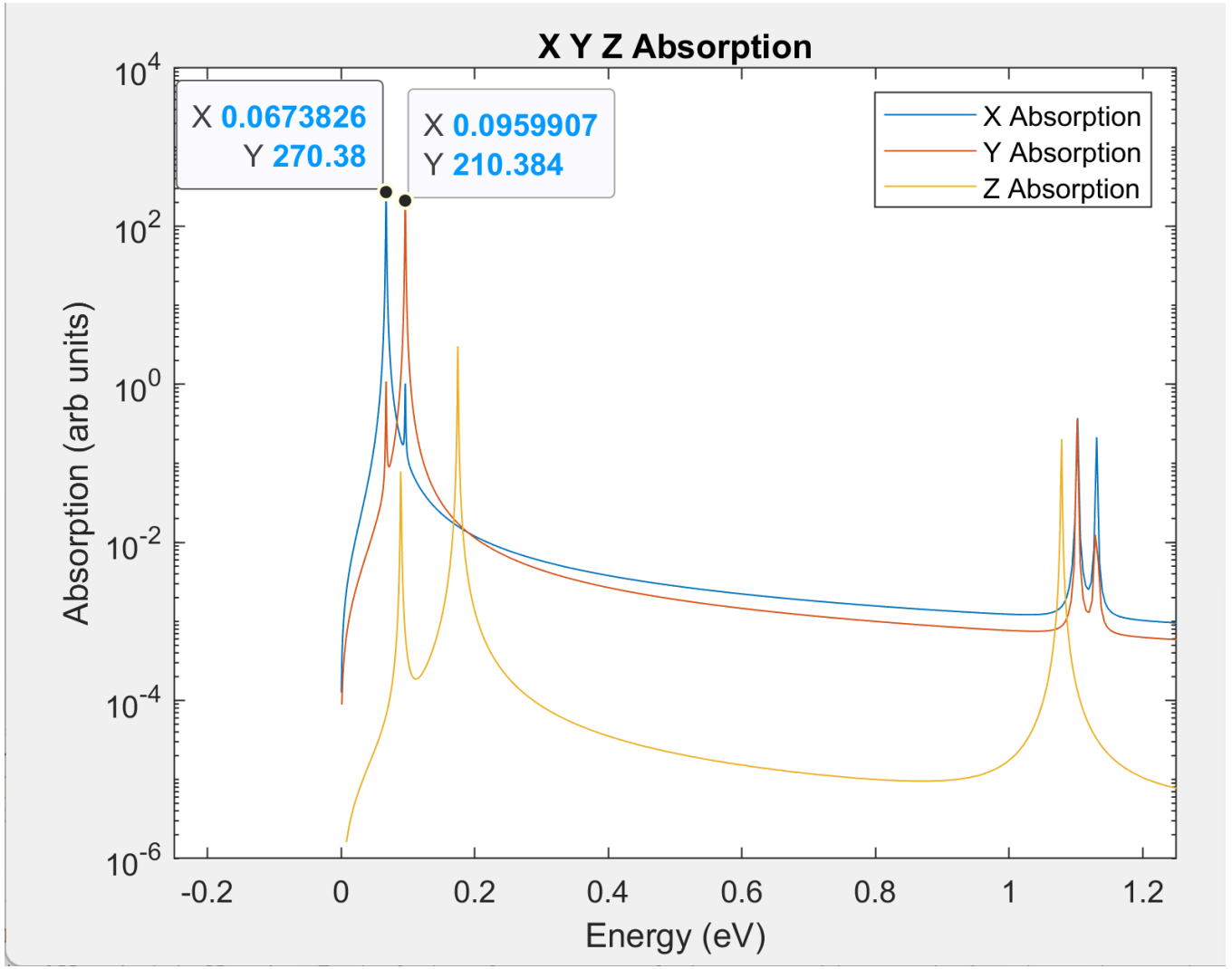
Additional Detail on Challenge 9 Solution

Inputs:

Structure: Dome

```
Quantum Dot:
X Dimension = 15nm
Y Dimension = 8nm
Z Dimension = 1.8nm

Optical:
Multilayer Fermi Level = 1.31eV
Temperature = 10K

Lateral Domain:
X Dimension = 20nm
Y Dimension = 20nm

Verticle Layers:
Substrate Z Dimension = 12nm
Wettin Layer Z Dimension = .3nm
Capping Layer Z Dimension = 2nm

Eigen Value:
Conduction Band: 1-1.6
Valence Band:-.5-1
```

Output:



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