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Quantum Dot Lab v. 2.0: Powered by NEMO 5

SURF
SUMMER UNDERGRADUATE RESEARCH FELLOWSHIPS

Lars Bjaalie
Network for Computational Nanotechnology (NCN)
Electrical and Computer Engineering
Klimeck Research Group
bjaalie@gmail.com

PURDUE
UNIVERSITY

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- Run the NanoHub.org tool "Quantum Dot Lab" with NEMO 5

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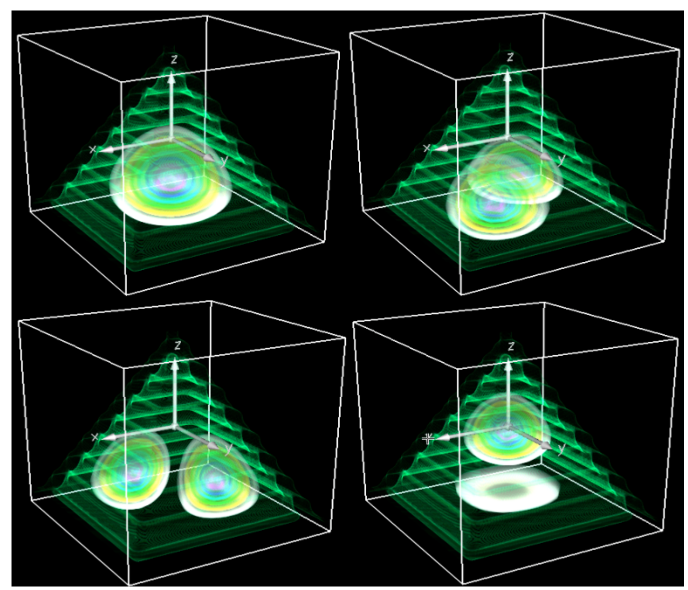

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What are Quantum Dots?

- Well conducting/low energy region surrounded within low conducting/high energy domain, on the nanometer scale
- Quantized electronic structure => “artificial atoms”
- So few electrons that what state individual electrons occupy become significant – a countable number of electrons
- Photon absorption: Detectors
- Photon emission: Lasers

Tailoring optical transitions!

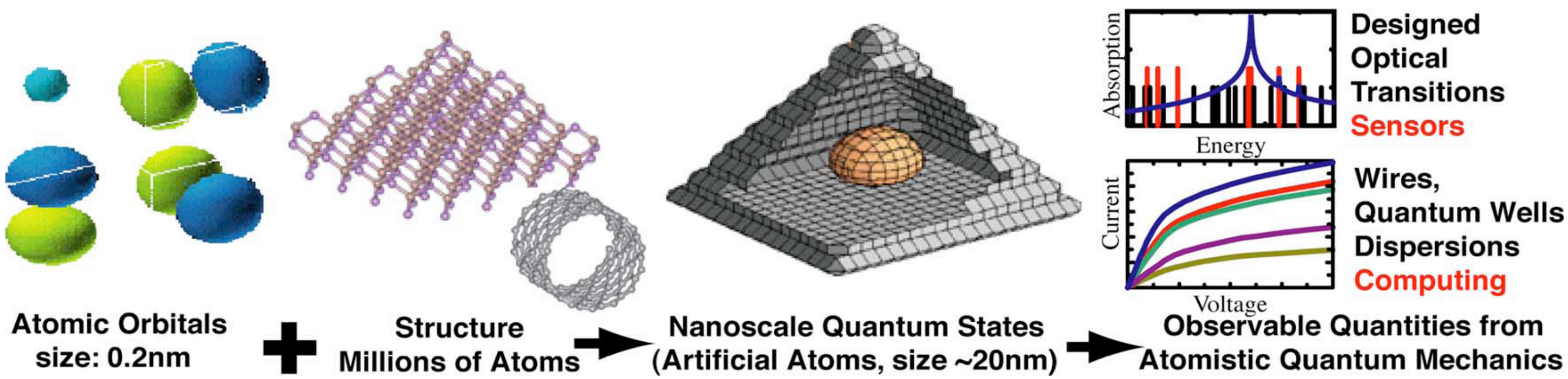


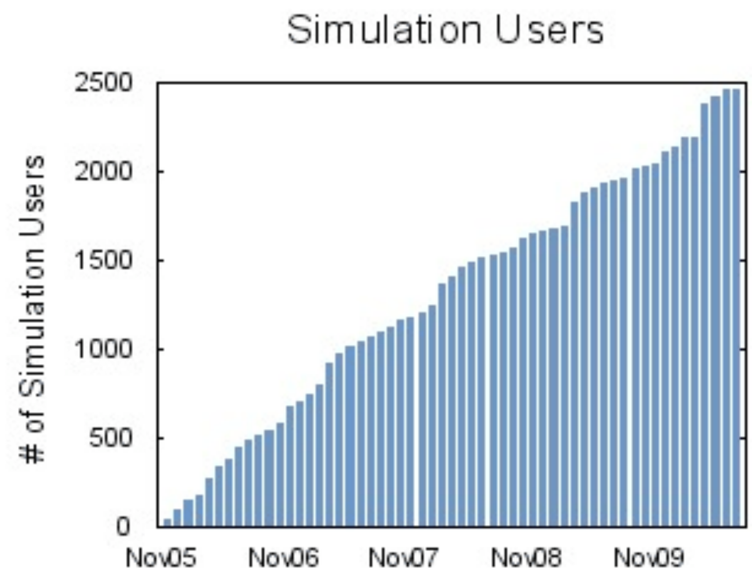
Image from “Atomistic simulation of realistically sized nanodevices using NEMO 3-D - Part I: Models and benchmarks”, IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. 54, NO. 9, SEPTEMBER 2007, G. Klimeck et. al.

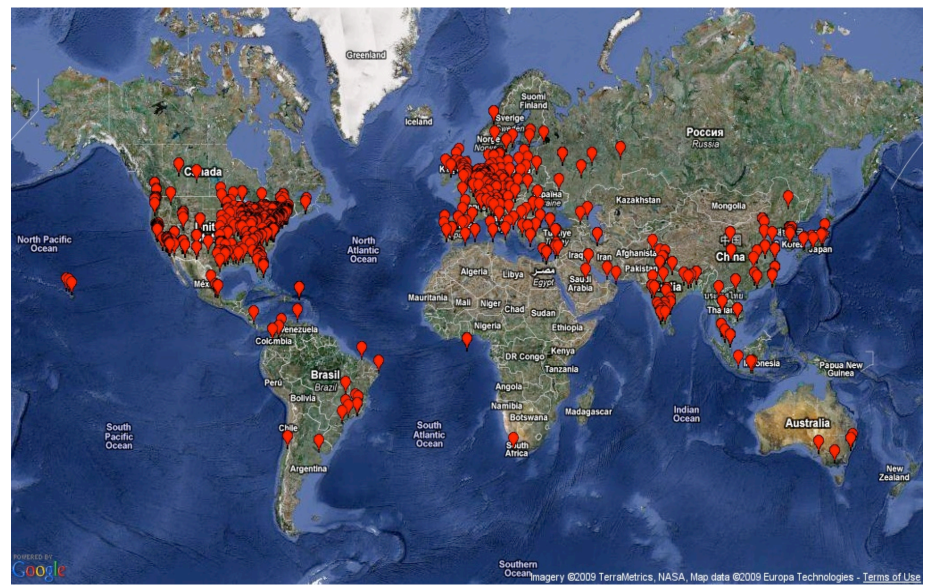
"Quantum Dot Lab" History and Usage

- One of the first tools on NanoHub.org
- Cited by 14 journal and conference papers
- Wide variety of teaching material based on the tool

Since its inception in 2005:

- 2500 simulation users
- 23,000 simulation runs
- 1.5 hours avg. interaction
- 83% educational use





NEMO 3-D vs NEMO 5

Problem in NEMO 3-D version of tool:

Incorrect physics => wrong energy levels

Energy level	Particle in a box (eV)	NEMO 5 (eV)	NEMO 3-D (eV)
1	2.10	2.24	2.21
2	2.77	3.02	4.36
3	3.44	3.79	6.51
4	3.89	4.17	7.75
5	4.11	4.56	8.67
6	4.56	4.95	9.91

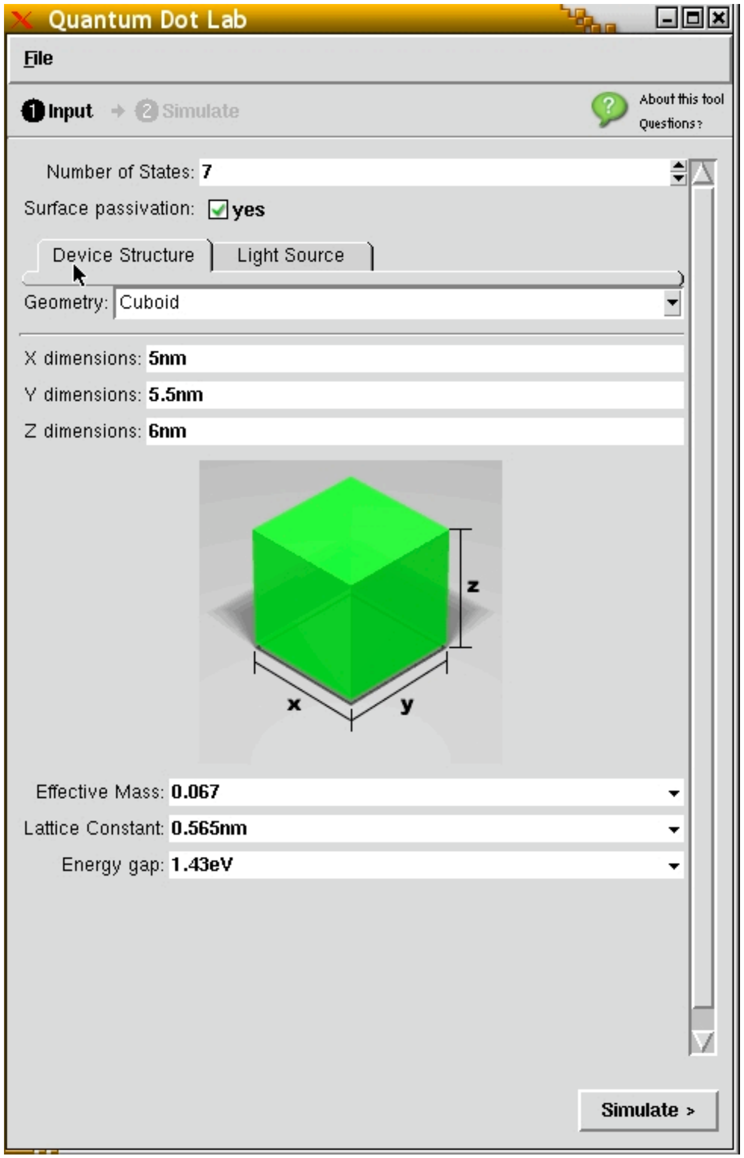
- NEMO 3-D difficult to edit
- NEMO 5 is under development

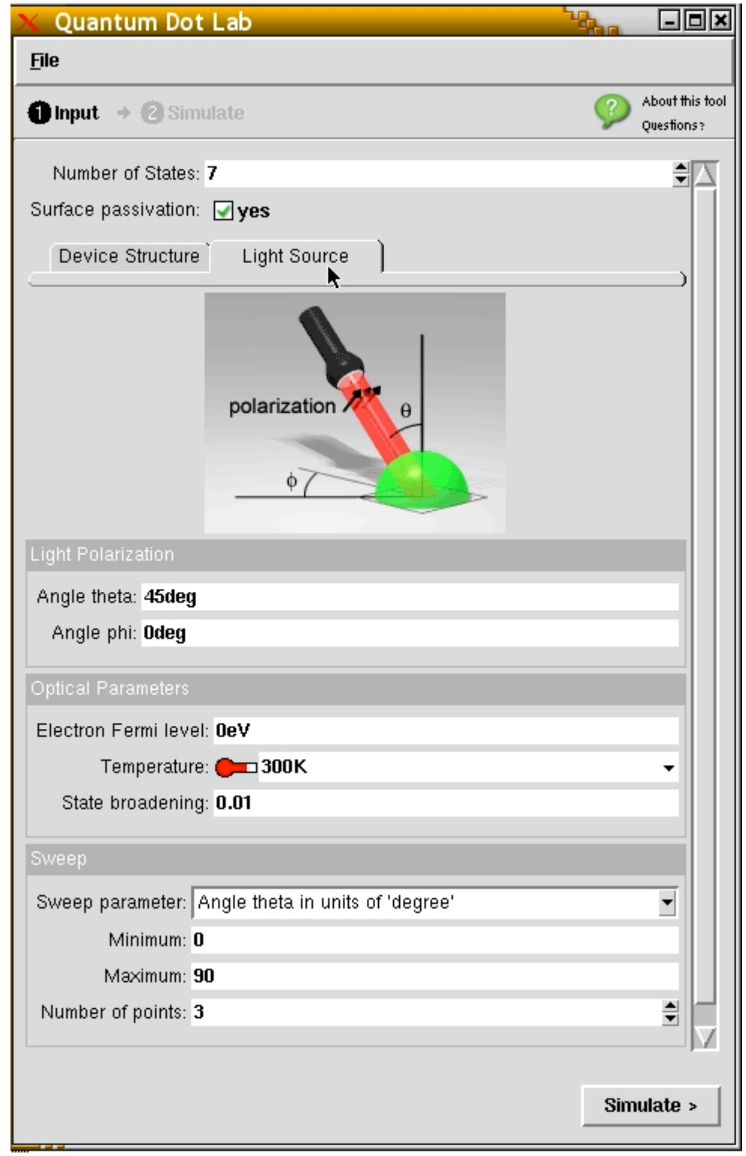
⇒ Implement correct physics in NEMO 5, to build a new tool

Missing NEMO 5 features

- Simple cubic crystal structure
- 1s tight-binding Hamiltonian
- Pyramid, spheroid, cylinder and dome geometries
- Open-DX wavefunction visualization
- Optical matrix elements
- Optical absorptions

Rappture Interface





1s Tight-Binding

- Matrix Schrödinger equation

$$E\vec{\psi}_{\vec{k}} = [h(\vec{k})]\vec{\psi}_{\vec{k}}$$

- Interaction matrix H_{nm} a scalar, only one wavefunction => one interaction

$$[h(\vec{k})] = \sum_m [H_{nm}] exp(i\vec{k} \cdot (\vec{d}_m - \vec{d}_n))$$

- Symmetry of simple cubic lattice gives an energy dispersion

$$E(\vec{k}) \approx E_0 + 6T - T(ka)^2$$

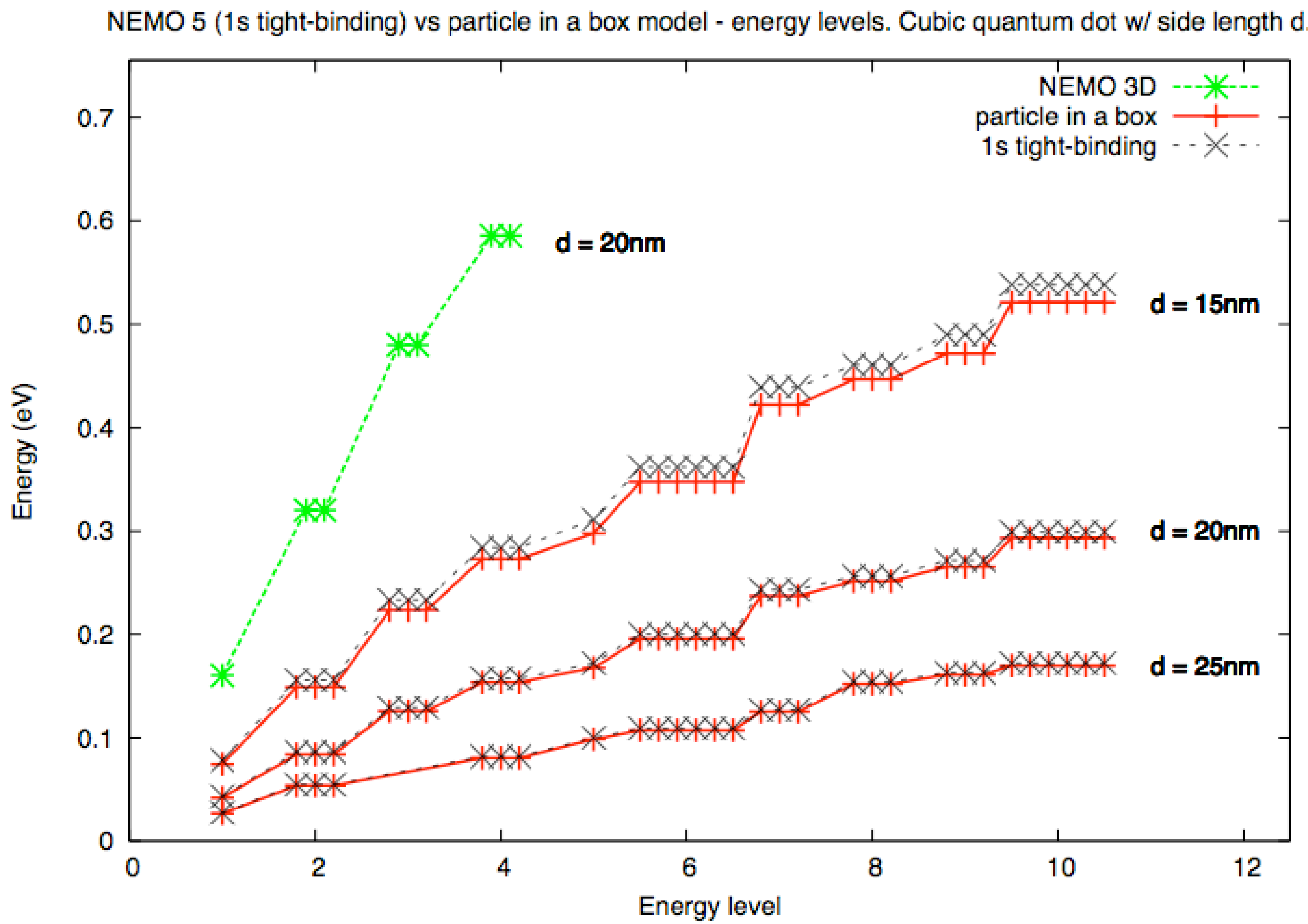
- Effective mass approximation gives E_0, T

$$\frac{1}{m*} = \frac{\partial^2 E}{\hbar^2 \partial k^2} = \frac{-2Ta^2}{\hbar^2}$$

- Need to solve the Hamiltonian matrix to find eigenvalues and eigenfunctions

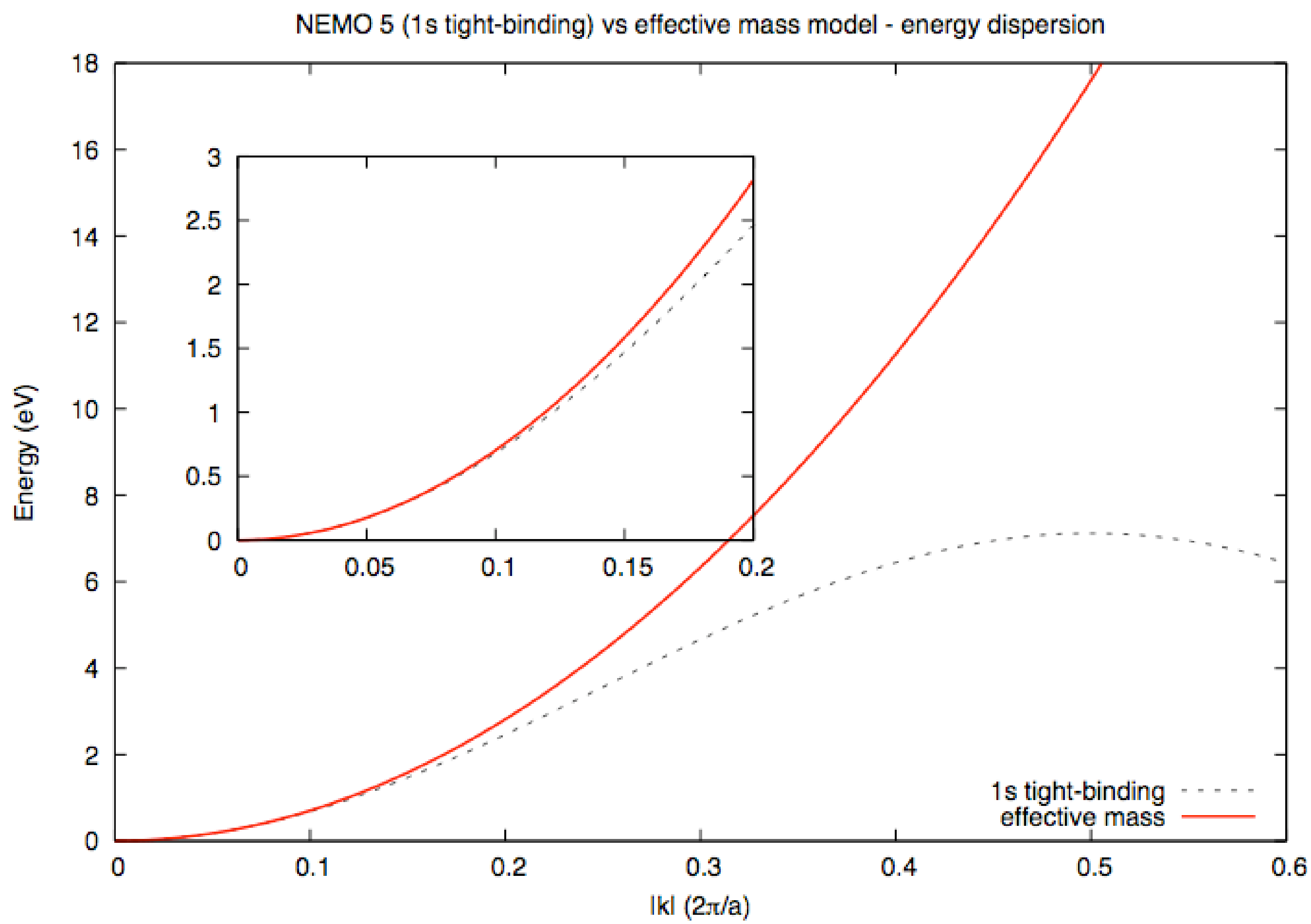
$$H = \begin{array}{c|cccc} & |1\rangle & |2\rangle & \cdots & |N\rangle \\ |1\rangle & E_0 & T & & 0 \\ |2\rangle & T & E_0 & & 0 \\ \vdots & & & \ddots & \\ |N\rangle & 0 & 0 & & E_0 \end{array}$$

1s Tight-Binding vs "Particle in a Box"



First 10 energy values for NEMO 5 (1s tight-binding model) and "particle in a box". An example from NEMO 3D shown for reference. Material parameters (effective mass and lattice constant) for GaAs.

1s Tight-Binding vs "Effective Mass"



Energy dispersion for NEMO 5 (1s tight-binding) and the "effective mass" model. Material parameters (effective mass and lattice constant) for GaAs. |k| normalized by $2\pi/a$, where a is the lattice constant.

Optical Absorption

- Fermi's golden rule for transition between two electronic states *a* and *b*

$$\frac{2\pi}{\hbar}|\langle b|H'(\vec{r})|a\rangle|^2\delta(E_b - E_a \pm \hbar\omega)$$

- Net upward transition rate (absorption)

$$\frac{2}{V}\sum_{\vec{k}_a}\sum_{\vec{k}_b}\frac{2\pi}{\hbar}|H'_{ba}|^2\delta(E_b - E_a - \hbar\omega)(f_a - f_b)$$

- Fermi function to account for occupancy of states

$$f_a = \frac{1}{1 + exp\left(\frac{E_a - E_F}{k_B T}\right)}$$

- Matrix elements give probability of transition

$$H'_{ba} \equiv \langle b|H'(\vec{r})|a\rangle = \int \Psi_b^*(\vec{r})H'(\vec{r})\Psi_a(\vec{r})d^3\vec{r}$$

Matrix Element Calculation

How do we calculate the matrix elements used in Fermi's golden rule?

- Electron-photon interaction Hamiltonian

$$H = \frac{1}{2m_0}(\vec{p} - e\vec{A})^2 + V(\vec{r})$$

- Light-perturbation part of Hamiltonian in terms of momentum matrix

$$H'_{ba} = -\frac{e}{m_0}\vec{A}\cdot\langle b|\vec{p}|a\rangle = -\frac{eA_0}{2m_0}\hat{e}\cdot\vec{p}_{ba}$$

- Ehrenfest's theorem to avoid calculating momentum matrix elements

$$\vec{p} = m_0\frac{\mathrm{d}}{\mathrm{d}t}\vec{r} = \frac{m_0}{i\hbar}[H,\vec{r}] = \frac{m_0}{i\hbar}(\vec{r}H_0 - H_0\vec{r})$$

- Calculate electric dipole moment instead

$$\langle b|\vec{p}|a\rangle = \frac{m_0}{i\hbar}\langle b|H\vec{r} - \vec{r}H|a\rangle = \frac{m_0}{i\hbar}(E_b - E_a)\langle b|\vec{r}|a\rangle$$

Optical Absorption- Final Expression

•Tight-binding wavefunctions are given in position representation => simple to calculate, sum over atomic positions i and orbitals j

$$\langle b|\vec{p}|a\rangle = \frac{m_0}{i\hbar}(E_2 - E_1)\sum_{ij}\psi_{ij}^{(b)*}\psi_{ij}^{(a)}\vec{R}_i$$

•Final expression for optical absorption, replace Dirac-Delta with Lorentzian

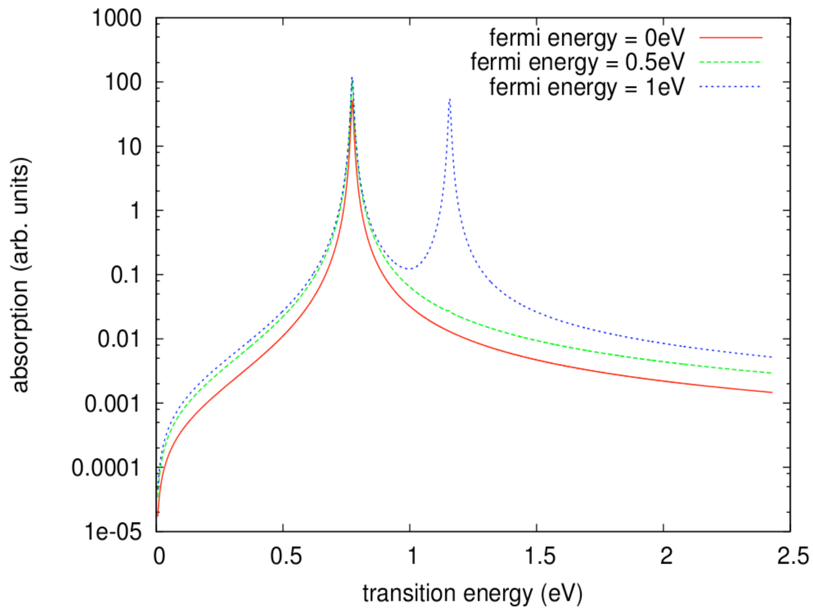
$$\alpha(\hbar\omega) \propto$$

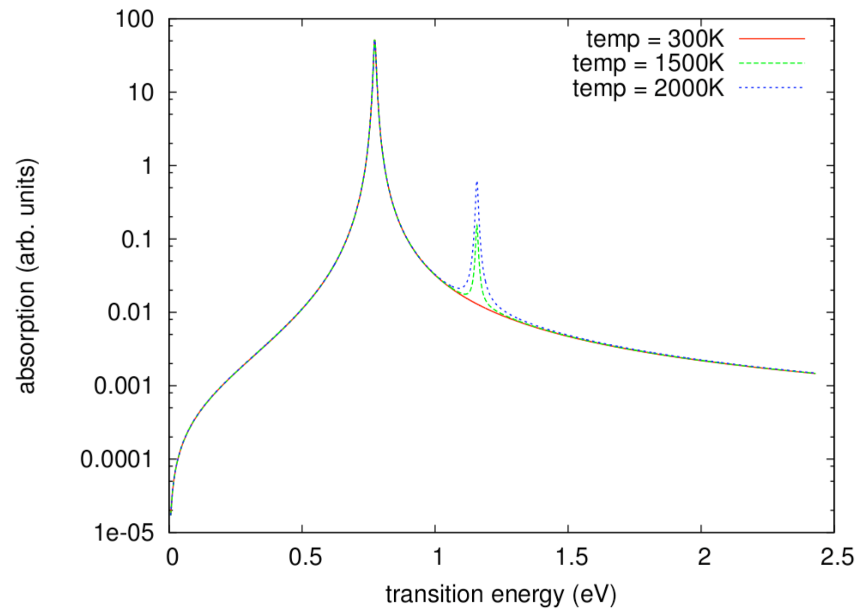
$$\left|\vec{e}\sum_{ij}\psi_{ij}^{(b)*}\psi_{ij}^{(a)}\vec{R}_i\right|^2 L(\Gamma, E_b, E_a, \omega)(f_a - f_b)$$

•Normalization and intensity dependence not included

$$L(\Gamma, E_b, E_a, \omega) = \frac{\Gamma/2}{(E_b - E_a - \hbar\omega)^2 + (\Gamma/2)^2}$$

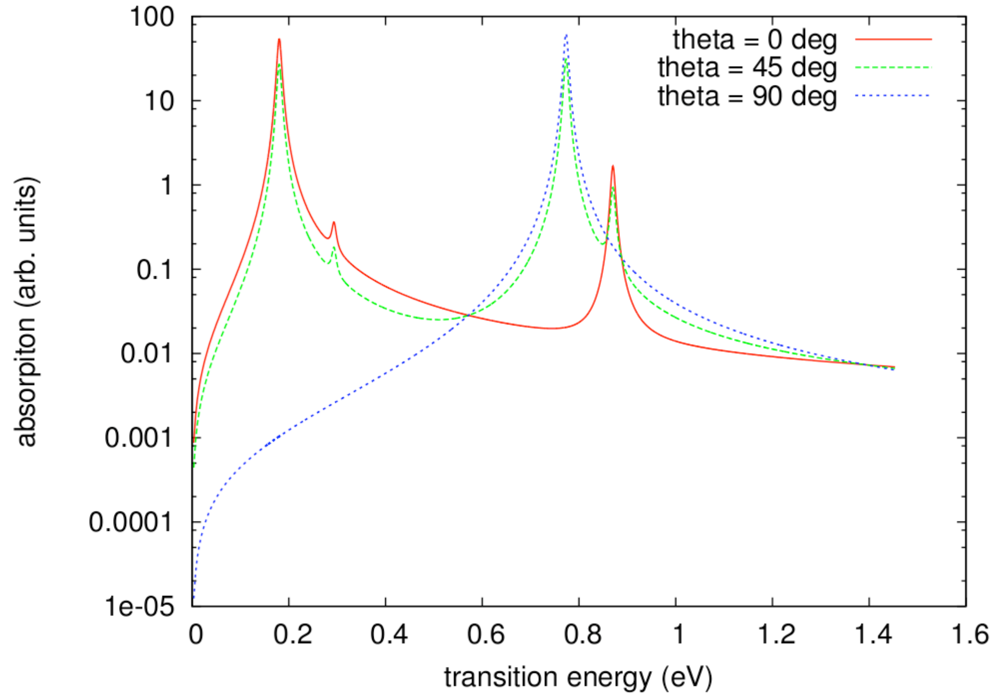
Absorption Plot - Fermi energy and temperature





5x5x5nm cuboid dot, keeping polarization angles constant. Raising the Fermi energy and temperature increases the occupation of higher energy states. Fermi level set at ground state energy. Calculation done with first 7 energy states. First peak between energy levels 1, and 2,3,4 (degenerate), second peak energy levels 7 and 2,3,4. Selection rules govern allowable transitions.

Absorption Plot – polarization angle



5x5x10nm cuboid dot, constant Fermi energy (0eV) and temperature (300K). Different light polarization emphasizes different transitions. Calculation done with first 7 energy states. First peak signifies absorption between energy levels 1 and 2, second 2 and 3, third 1 and 4, 5 (degenerate), fourth 1 and 6. Selection rules govern allowable transitions.

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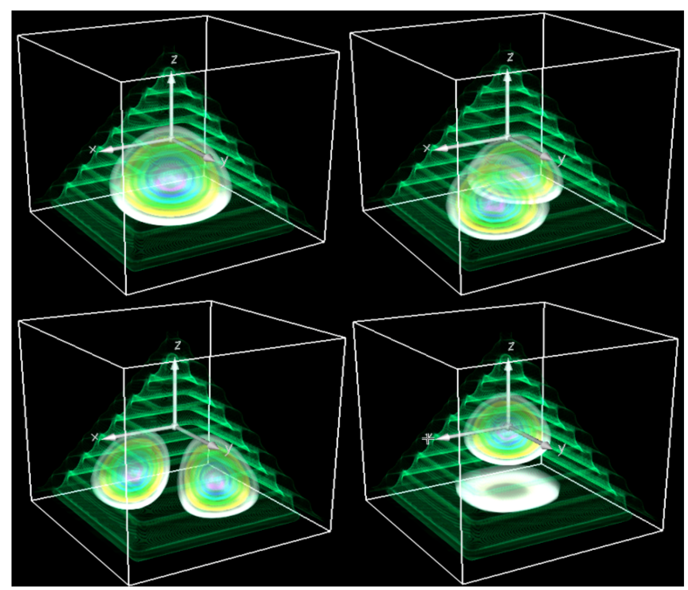

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Future Work / Acknowledgments

- Tool was redone to replicate the functionalities of previous tool, to keep in line with learning material
- Expert "Quantum Dot Lab" tool a possibility, including more electronic structure models (sp3s* or sp3d5s* tight binding, k.p theory, including spin)
- Upload on NanoHub.org!

- Klimeck research group: Sebastian Steiger, Parijat Sengupta, Michael Povolotskyi, Tillmann Kubis, Prof. Klimeck
- SURF program and Purdue University for providing a stipend for the summer
- NCN for hosting summer interns

NEMO 3-D vs NEMO 5

- NEMO: NanoElectronic MOdelling tool
- Multimillion atomistic tight -binding simulations

- "Quantum Dot Lab" will be first showcase of NEMO 5 on NanoHub.org

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- NEMO 3-D: Written in C

Functions to calculate matrix elements and absorptions in opt3d.c

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Called in nemo3d_entry.c, depending on input

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Simulation run in run3d.c

NEMO 5: Written in C++

Classes **MatrixElementCalculator** and **Absorption** handle the physics

↓

Class **MatrixElements** handles input, calculations, and output

↓

Class **Nemo** runs simulation