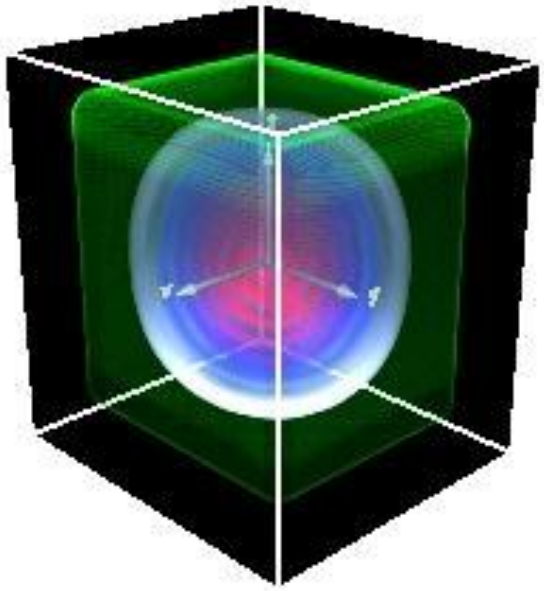
NCN

First-Time User Guide for Quantum Dot Lab*



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*http://www.nanohub.org/tools/qdot/.

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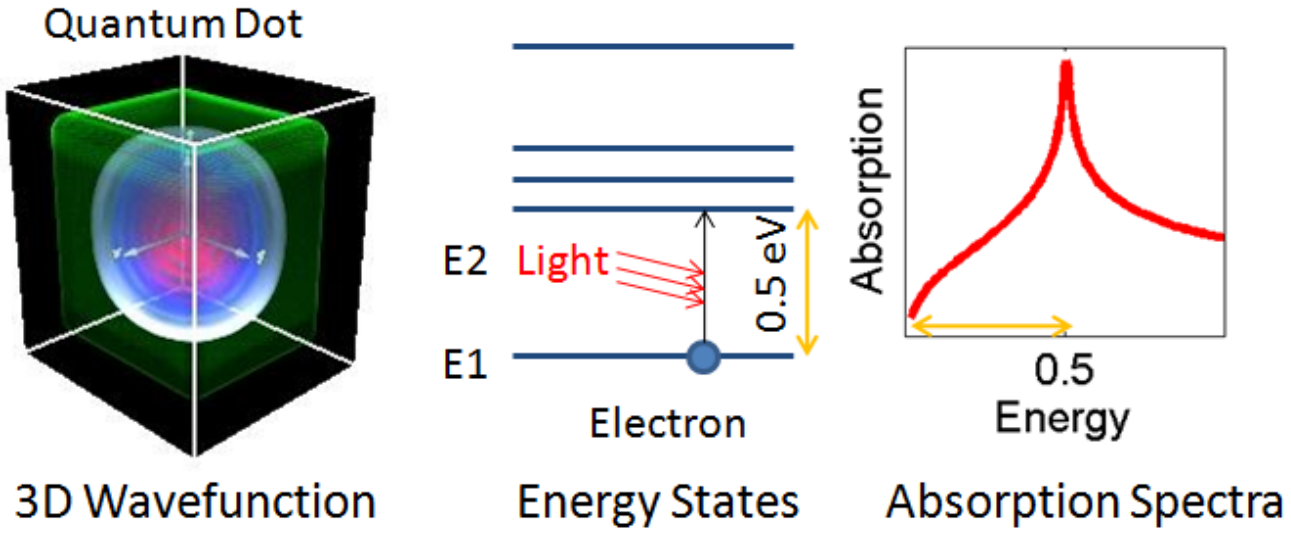
Introduction

- The quantum dot lab is a tool that solves the Schrödinger equation for an electron in a quantum dot.
- The quantum dot lab yields the wavefunction, the electron energy levels, and the optical transition rates/absorption strength of an electron.



A detailed introduction to the quantum dot lab also can be found at https://www.nanohub.org/resources/4194.

First Look

1 Input → 2 Simulate

About this tool
Questions?

Number of States: 7

Surface passivation: "yes"

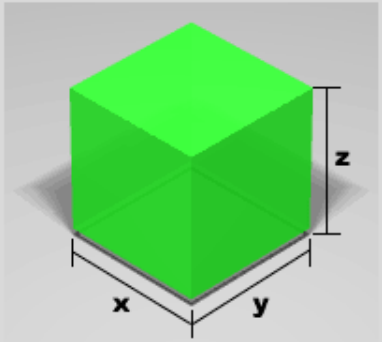
Device Structure | Light Source

Geometry: Cuboid

X dimensions: 10nm

Y dimensions: 10nm

Z dimensions: 10nm



Effective Mass: 0.067

Discretization: 0.565nm

Energy gap: 1.43eV

Simulate >

Input Interface

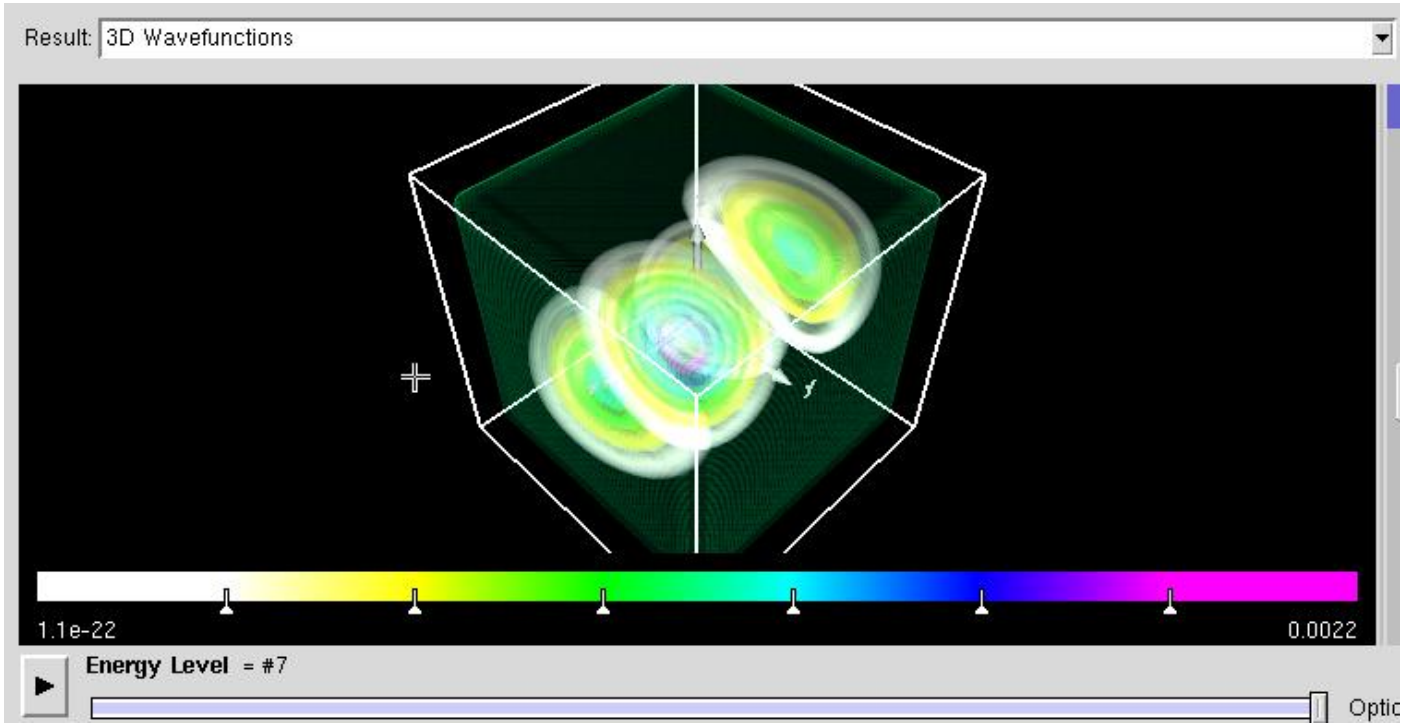
- Number of states
- Device structure
  - » geometry
  - » effective mass/ discretization/ energy gap
- Light source
  - » light polarization
  - » optical parameters
  - » sweep

The Number of States

- First, choose the number of states: the default value is “7.”

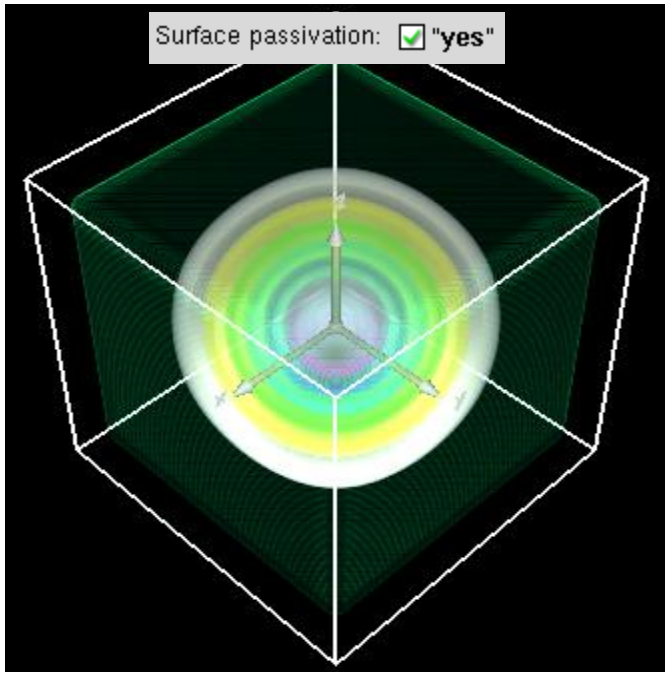
Number of States: 7

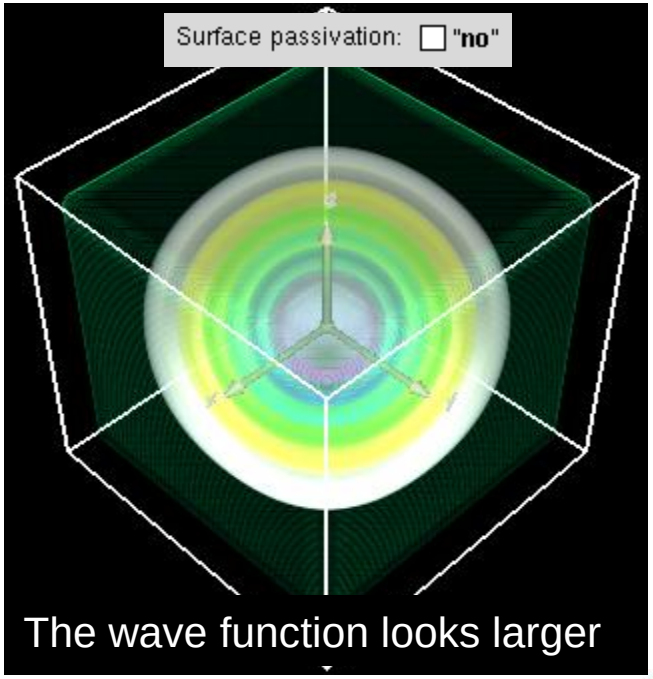
- How many states do you want to see in the output?
  - » Do not choose an unnecessarily large number; it increases the run time.
- The output below shows that up to 7 energy levels are viewable, if the number of states chosen in the input is 7.



Surface Passivation

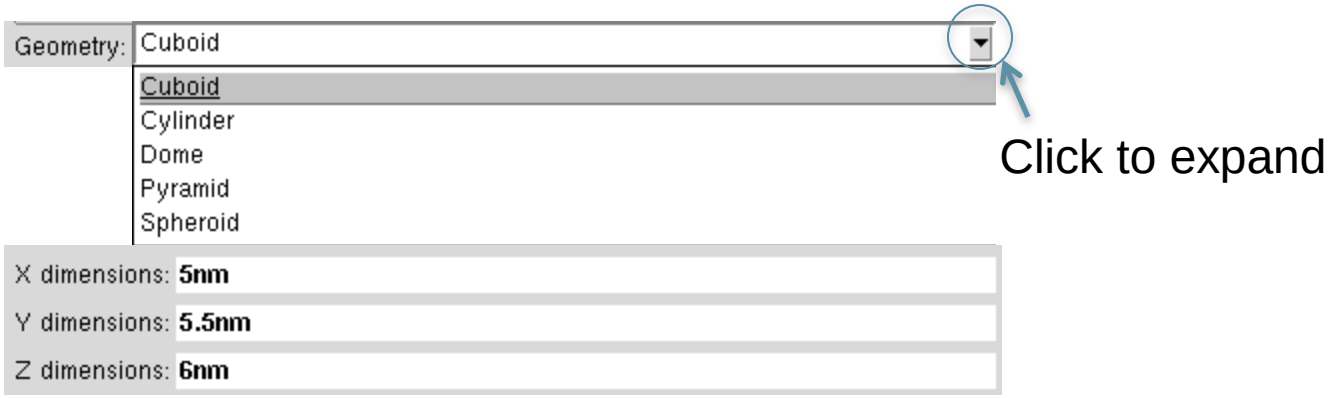
- The “surface passivation” option passivates the surface so that the electron feels an infinite potential barrier at the surface of the quantum dot.
  - » Surface passivation forces the electron wave function at the surface of the quantum dot to go to zero.
  - » If “no” is chosen, then the wavefunction is allowed to leak out of the quantum dot. The result is illustrated in the following figures:

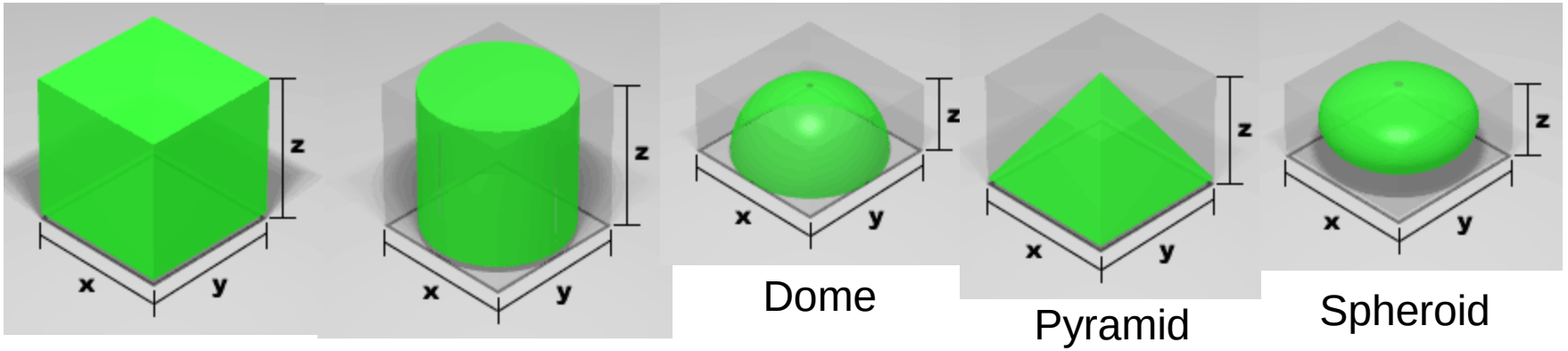




Device Structure: Geometry

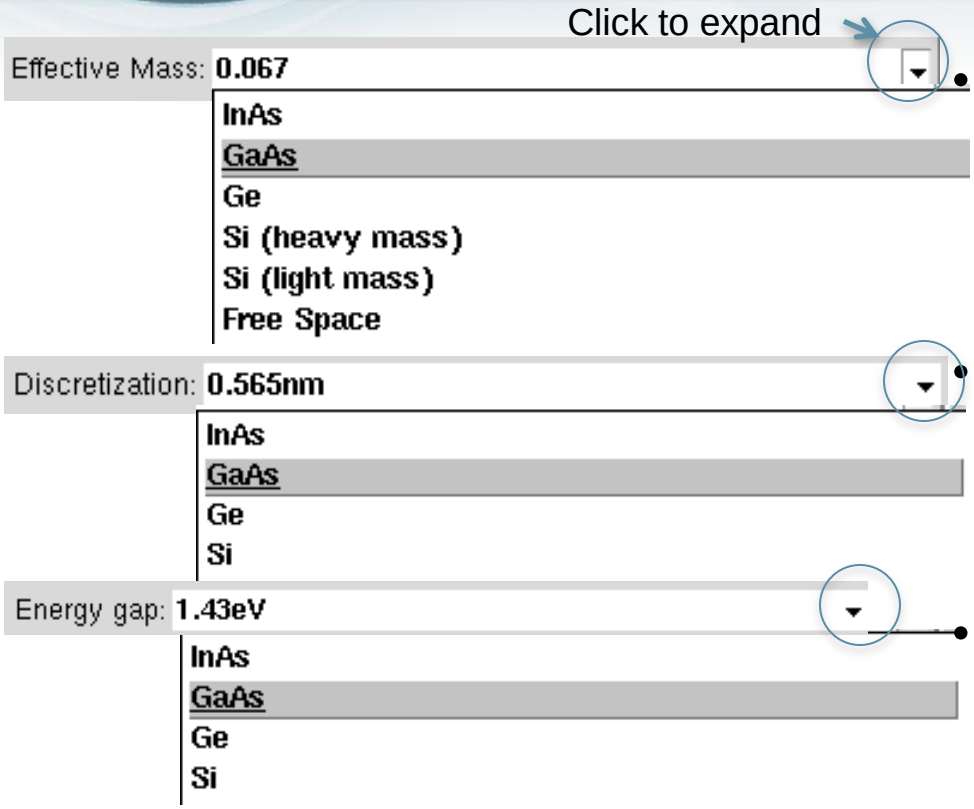
- The geometry can be set by choosing x, y, and z dimensions for each of the configurations shown below.





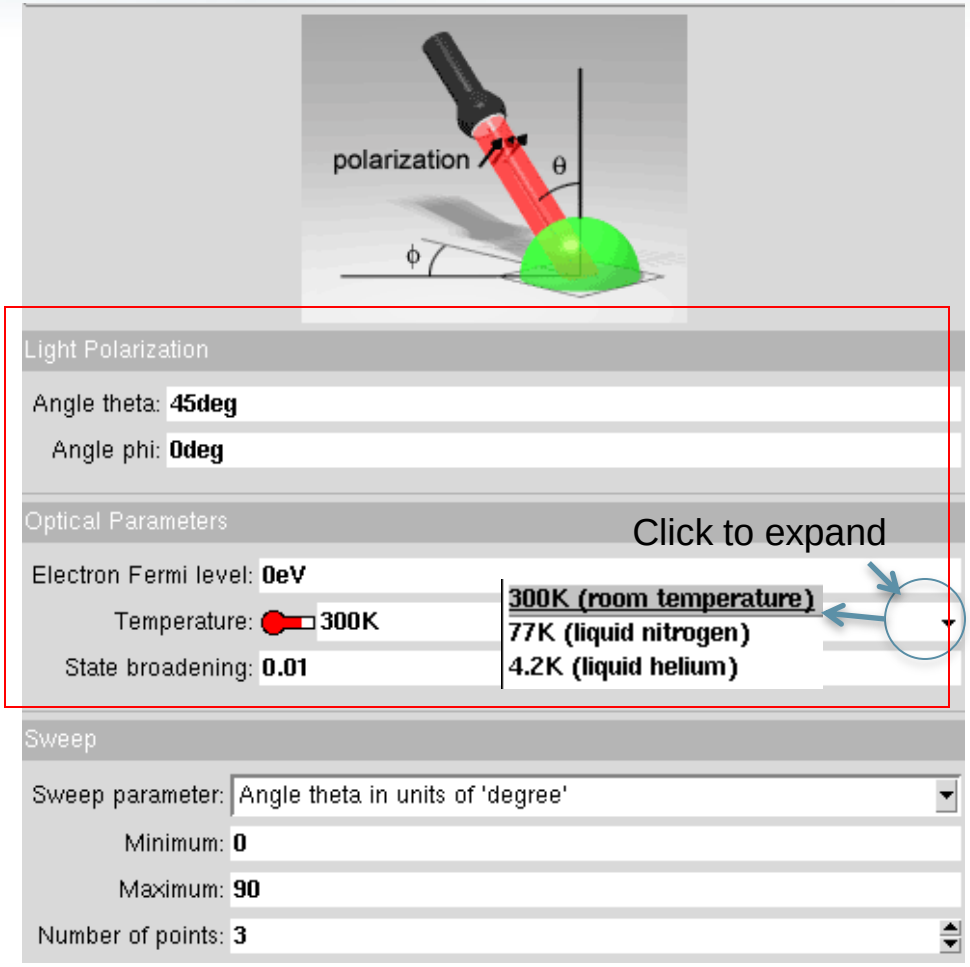
Cuboid Cylinder Dome Pyramid Spheroid

Other Device Structure Parameters



- Effective mass
  - » Ratio to the free electron mass (m_0)
  - » e.g., 0.067 means $m = 0.067 \times m_0$
- Discretization
  - » The discrete mesh spacing in the quantum dot domain (simple cuboid for all shapes of quantum dot)
- Energy gap
  - » The energy gap between the valance and the conduction band edge

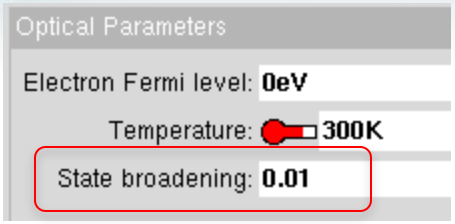
Light Source: Polarization/Optical Parameters

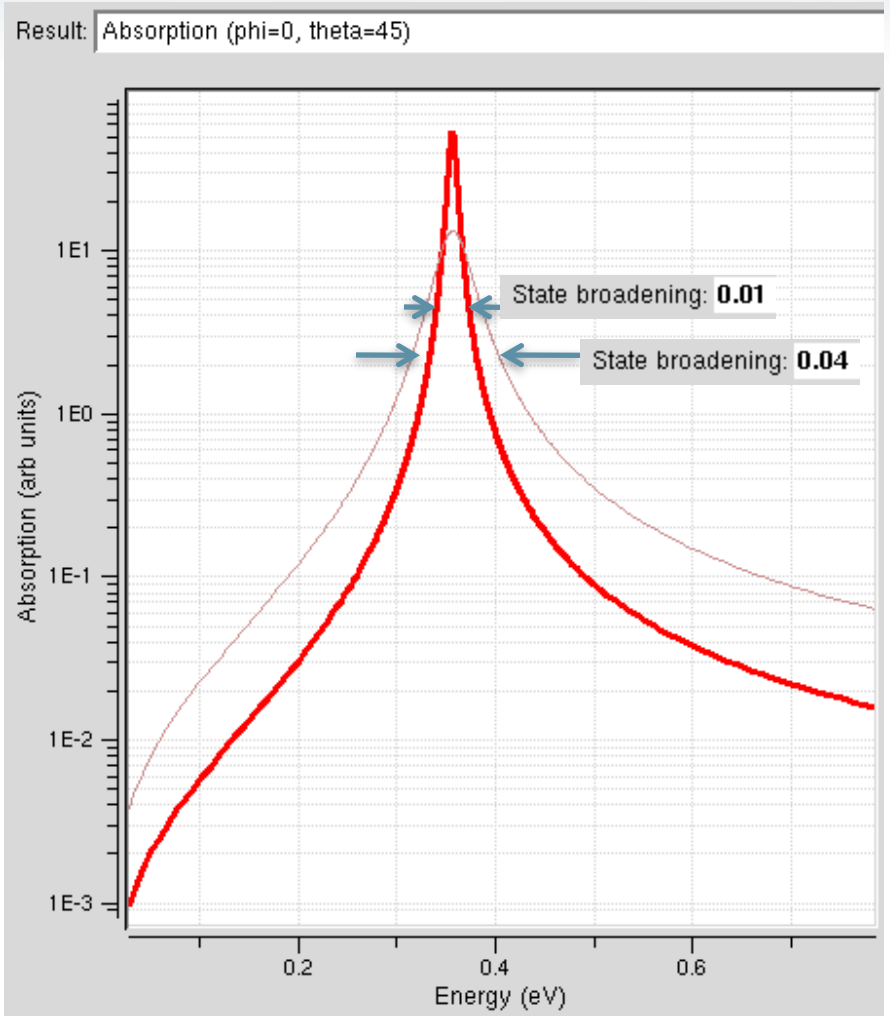


- The light source shines on the quantum dot to reveal the optical properties.
- Users can choose the angles *theta* (θ) or *phi* (Φ) as shown in the figure to the top left.
- Fermi level (relative to the lowest energy level)
- Temperature (ambient temperature)

For a detailed description, see: https://www.nanohub.org/resources/4194

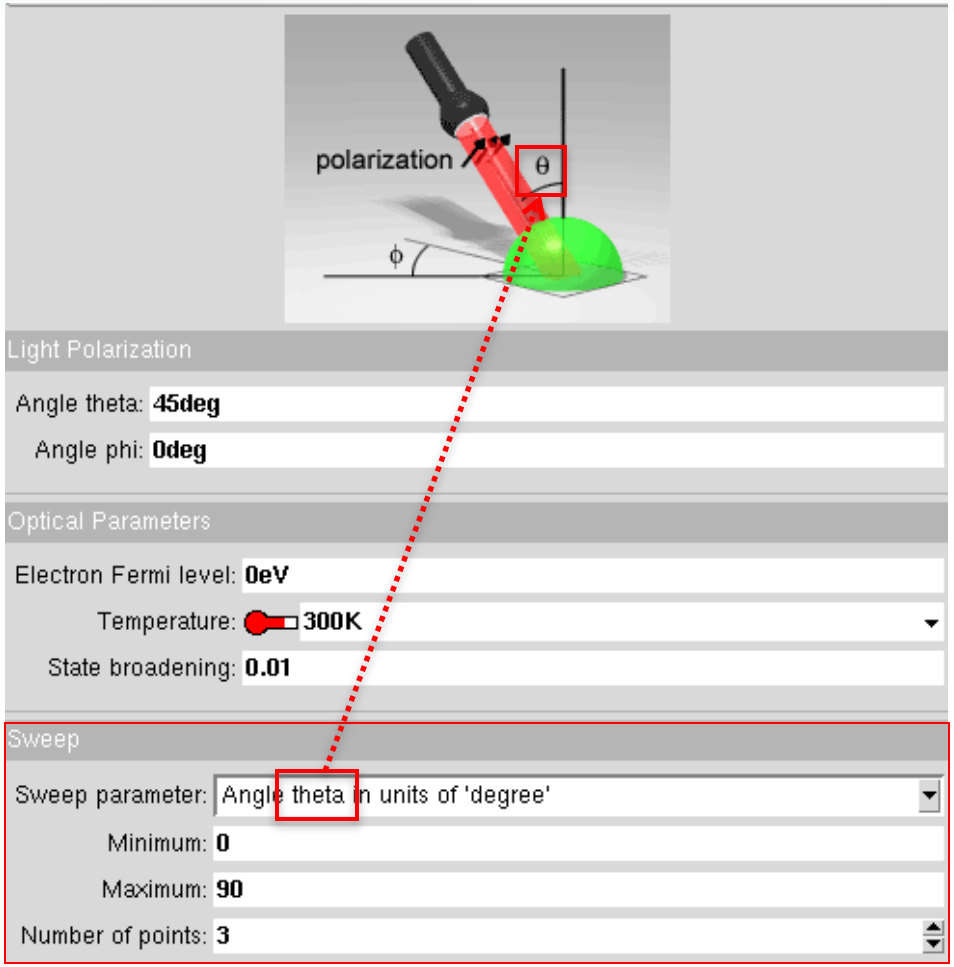
Light Source: State Broadening

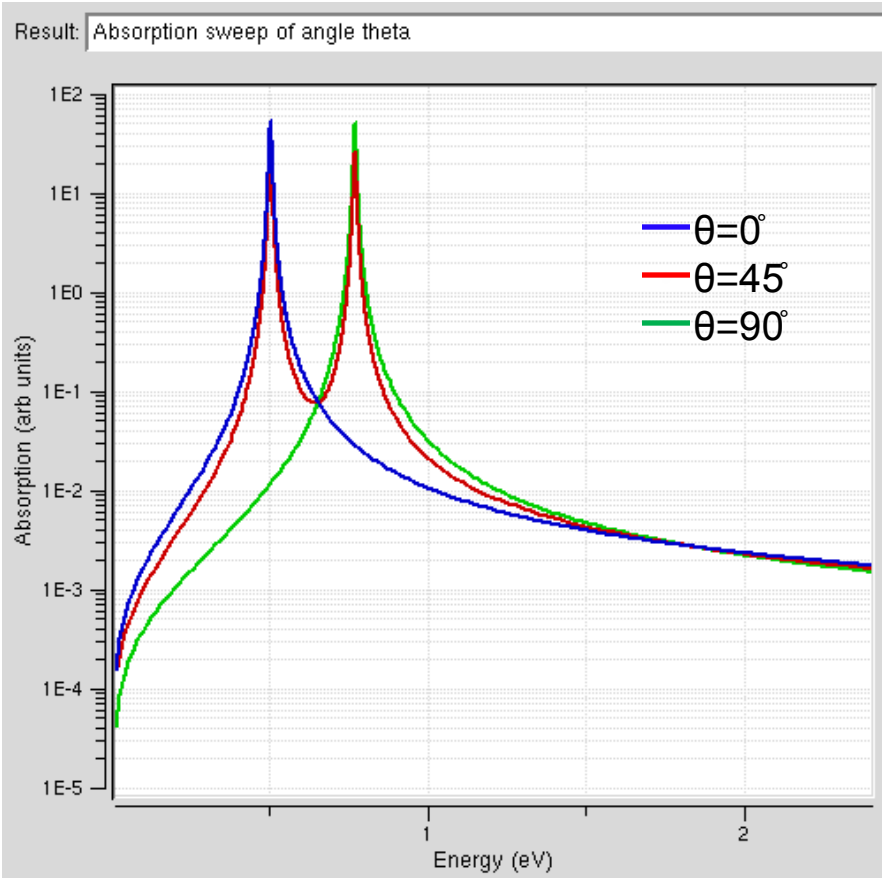




- "State broadening" determines:
  - » the broadening width of the energy states in the quantum dot
  - » the width of the Lorentzian shape of the optical absorption

Light Source: Sweep





Output Interface

- **3D wavefunctions**: 3D plot of the electron wavefuction in a quantum dot
- **Energy states**: the energy levels of the electron in a quantum dot

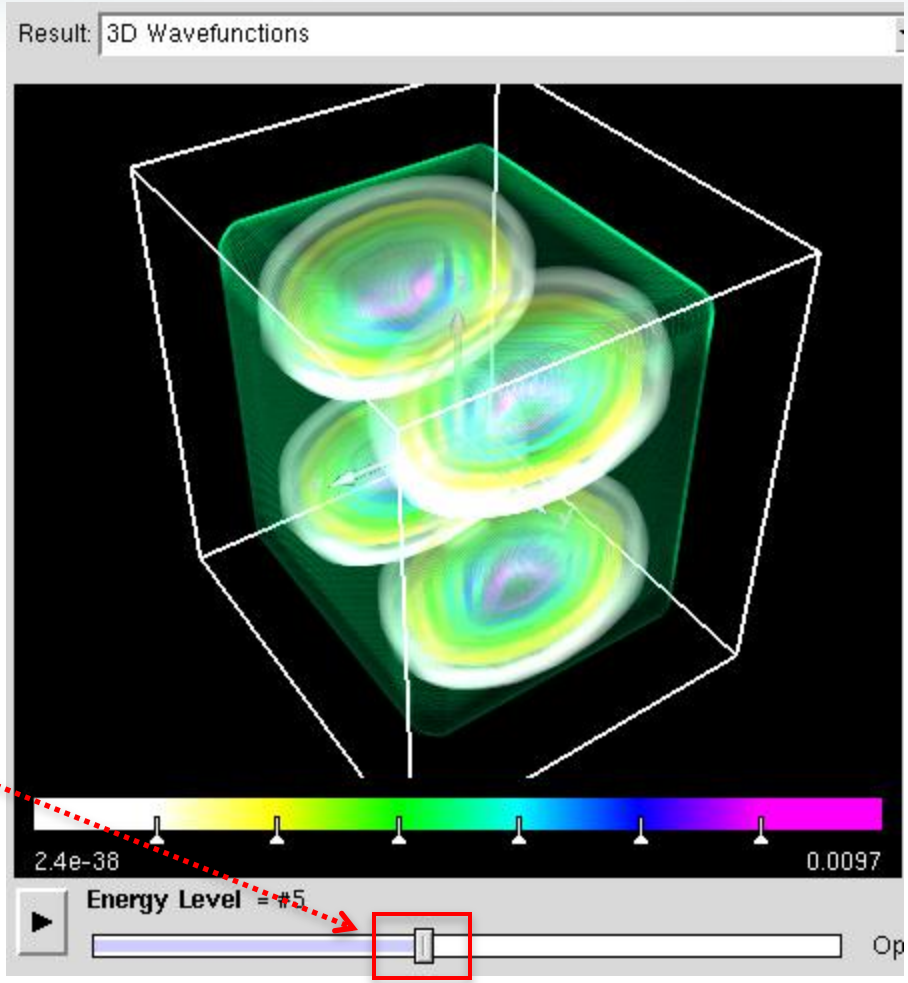
Optical Properties

- **Light and dark transitions**: the transition strength of electrons when the light shines onto a quantum dot
  - » X-polarized: when X-polarized light is shined
  - » Y-polarized: when Y-polarized light is shined
  - » Z-polarized: when Z-polarized light is shined
- **Absorption**: the absorption strength
- **Absorption sweep**: the absorption strength plot when the angles *theta*, *phi*, Fermi level, or temperature is swept.
- **Integrated absorption**: the integrated (the area under the graph of) absorption for each sweeping variable.

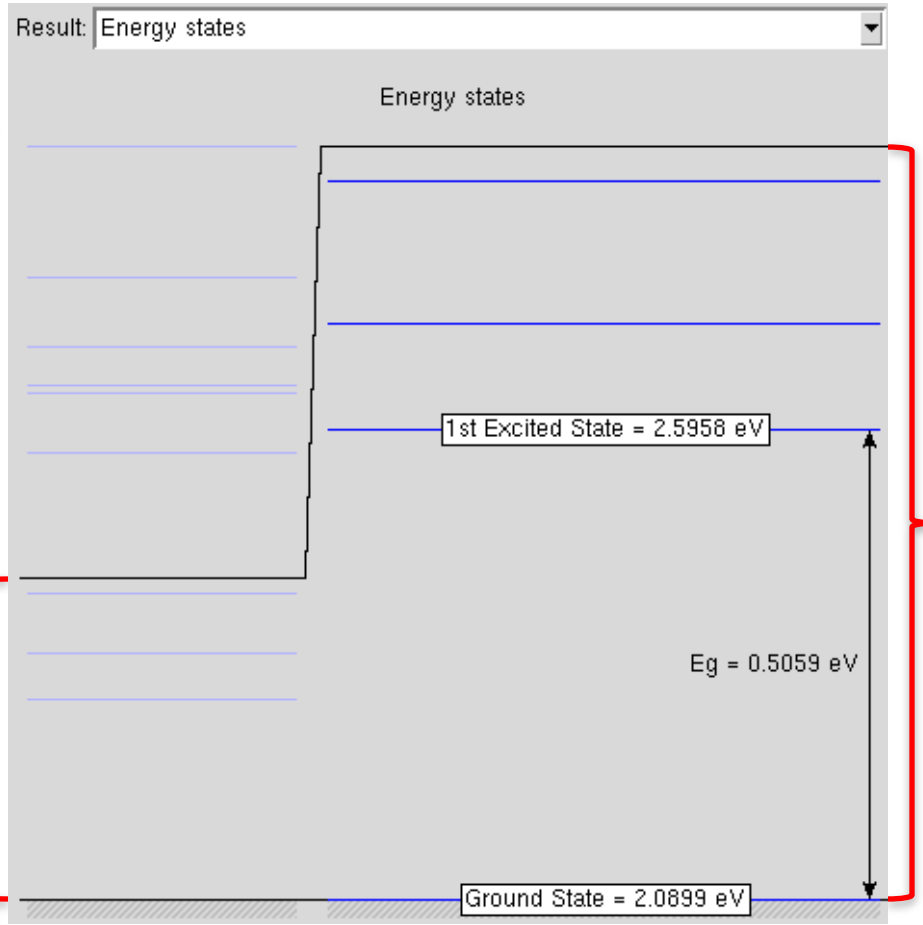
Refer to the introductory tutorial for more examples of the optical properties
https://www.nanohub.org/resources/4194

3D Wavefunctions

Use this tab to explore different energy states



Energy States



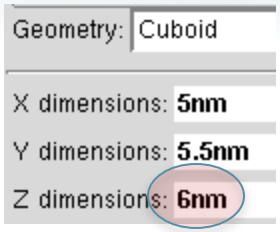
Total energy range

Energy range selected

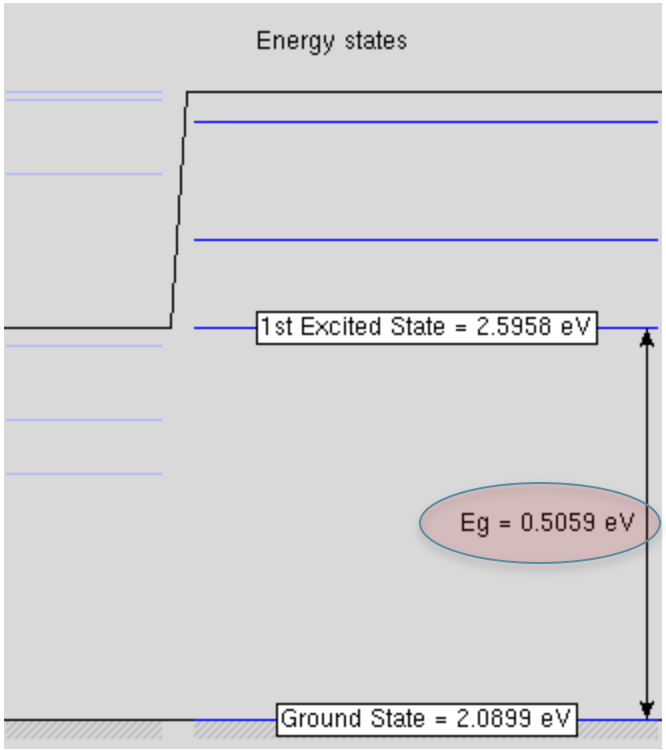
States Order	Notations in Qdot Lab
1st state	Ground state
2nd state	1st excited state
3rd state	2nd excited state
…	…

Magnified view of the selected portion

Optical Properties: Transition Strength



From the geometry, expect that the p_z–type orbital has the lowest energy. (Inverse order to the real space dimensions.)



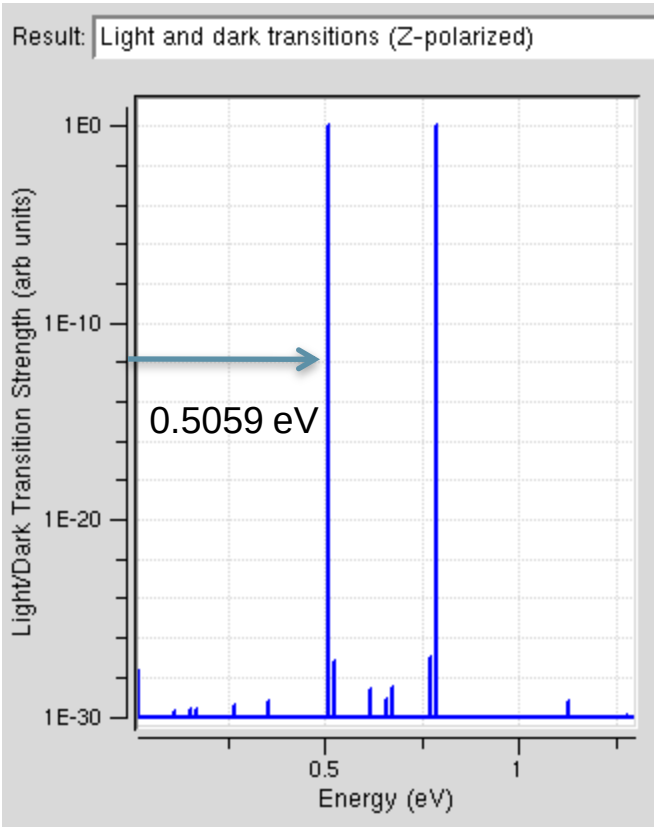
p_x

p_y

p_z

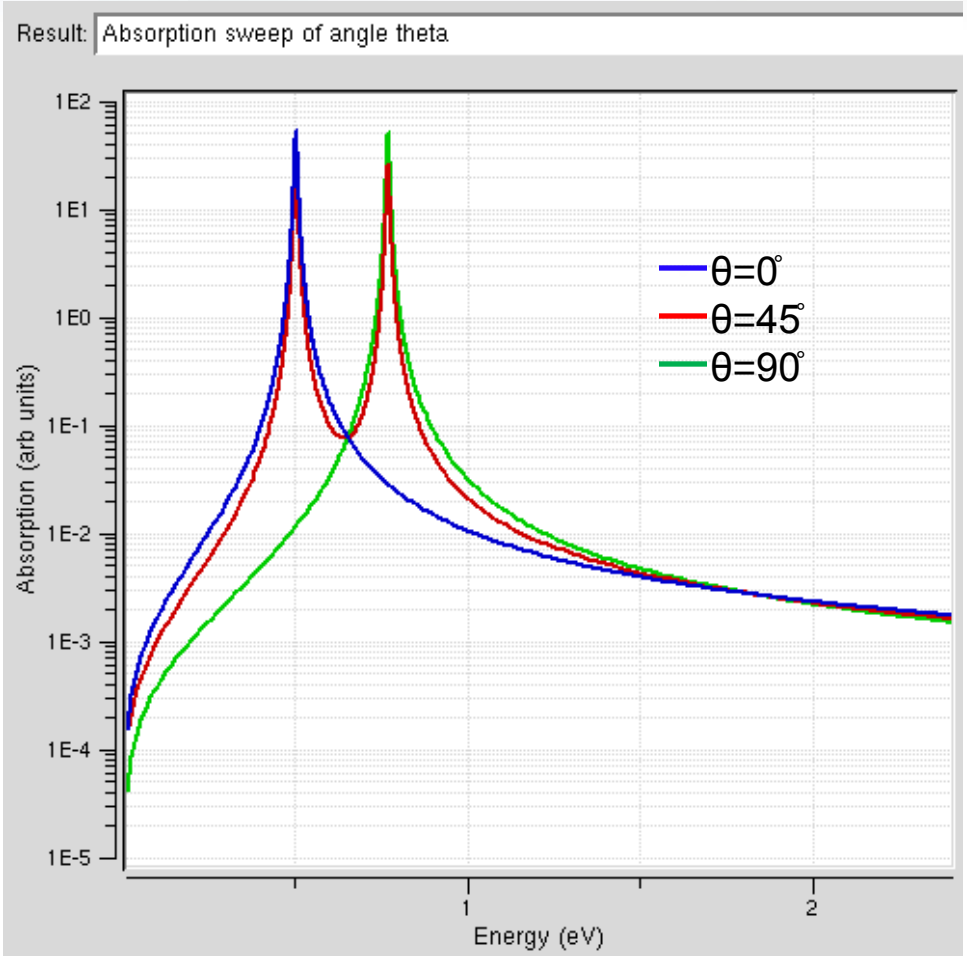
s

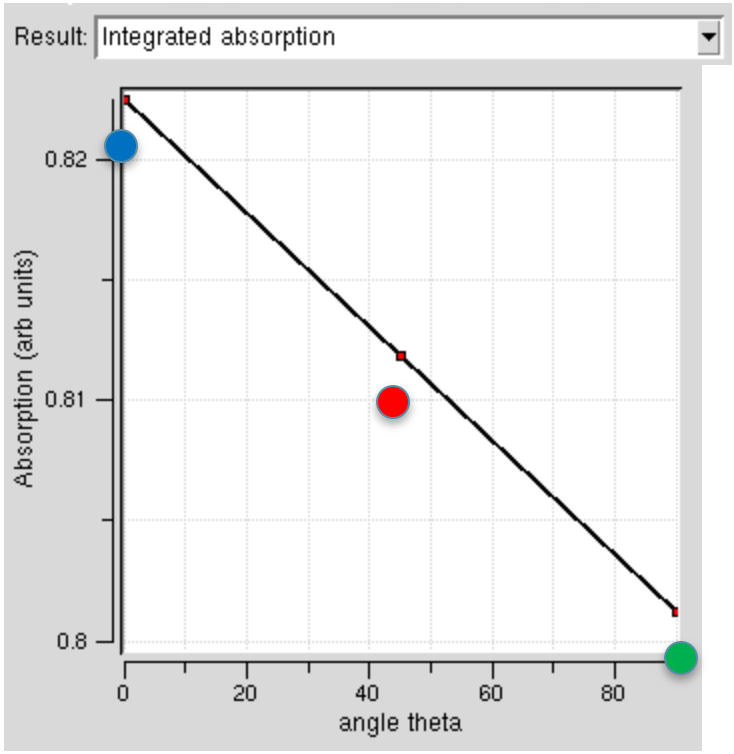
s to p_z orbital transition can be observed by <u>Z-polarized light</u>



The first large transition comes exactly at the transition energy from s to p_z type orbital.

Optical Properties: Absorption





Each point is calculated by integrating each absorption graph (note that the color of each point matches the color of the line in the left figure).

Simulation Engine Behind the Tool: NEMO 5

- Right now, the engine for the quantum dot lab is NEMO 5.
- NEMO 5 is a Nano Electronic MOdeling tool.[2]
- The quantum dot lab tool mainly uses the following parts of NEMO 5:
  - » structure construction
  - » Schrödinger solver
  - » optical properties solver

[2] https://engineering.purdue.edu/gekcogrp/research-group/SebastianSteiger/quad_NEMO5.pdf

References

[1] Gerhard Klimeck, Introduction to Quantum Dot Lab: https://www.nanohub.org/resources/4194

[2] Sebastian Steiger, NEMO 5 quad chart: https://engineering.purdue.edu/gekcogrp/research-group/SebastianSteiger/quad_NEMO5.pdf