Review of Group Project

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Friday 10th May, 2013

1 Done so far...

- Simulation procedure automatized
- Build a DB with simulation data
- *Toolbox* to visualize the simulation data

2 Outlook

- Poster of Quantum Dot & Solar Cell processing
- Documentation: Interpreting results, MATLAB

3 Questions

- Difference Quantum Dot & Nanocrystal? (Semiconductor nanocrystals in the sub-10 nm size range are often referred to as quantum dots)?
- Simulation of other materials?
- What is the date of the presentation?
- Need more disc space.
- How relevant is MATLAB work, are the Simulation data?
  - → Storage on a server?
  - → Documenting MATLAB work (User, Maintainer)?
  - → Installer for scripts and functions (*Toolbox*)?

4 Some Examples of the Simulation Results

4.1 Quantum Dot Structure

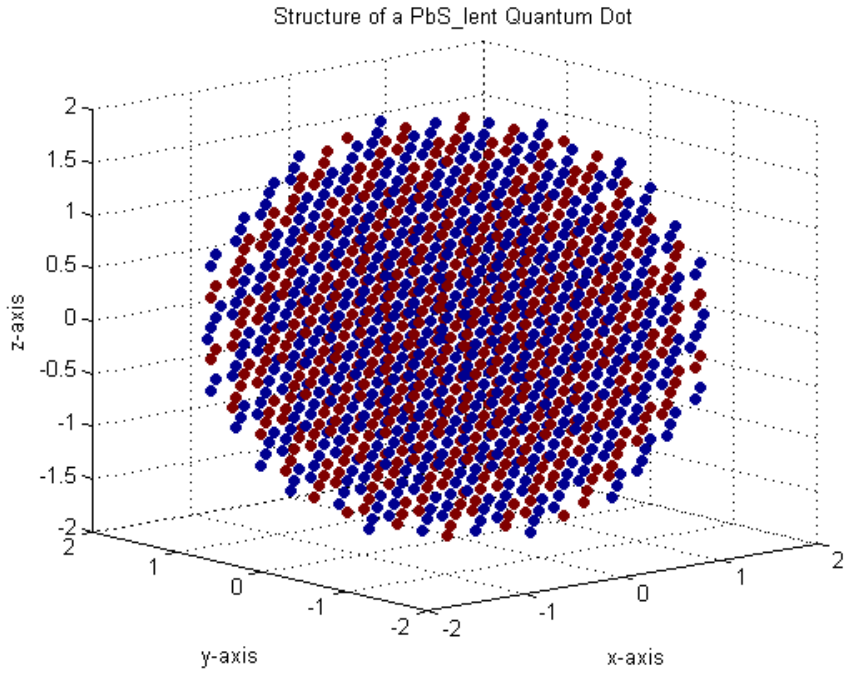

Figure 1: Atomic Structure of a PbS Quantum Dot of 4nm diameter

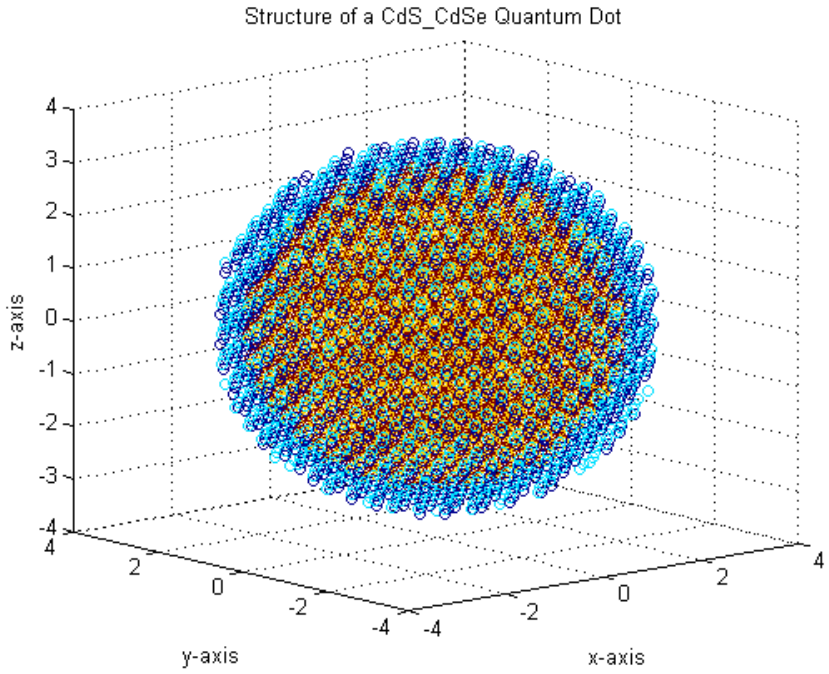

Figure 2: Atomic Structure of a CdSe-CdS Quantum Dot with 6nm core diameter (CdSe) and a 7nm shell diameter (CdS)

4.2 Wavefunctions

Wavefunctions of different radii

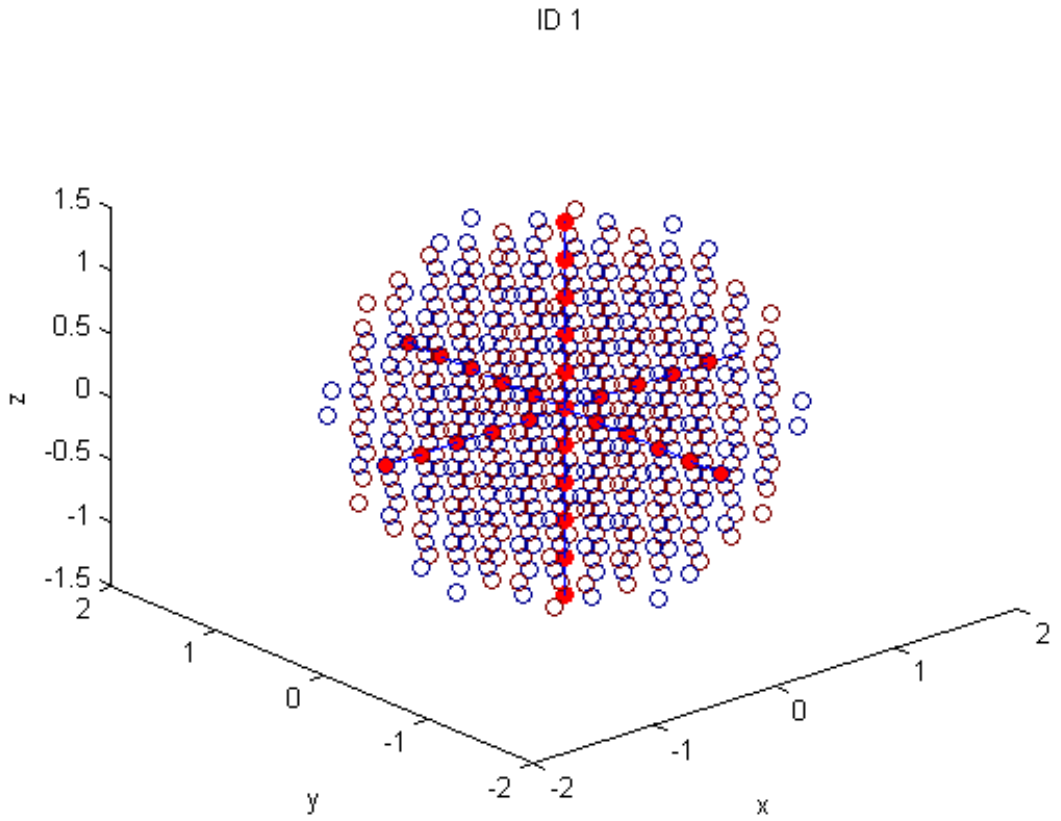

Figure 3: Quantum Dot structure showing axes along which wavefunctions are plotted. Red dots are atoms that are taken into account for the function

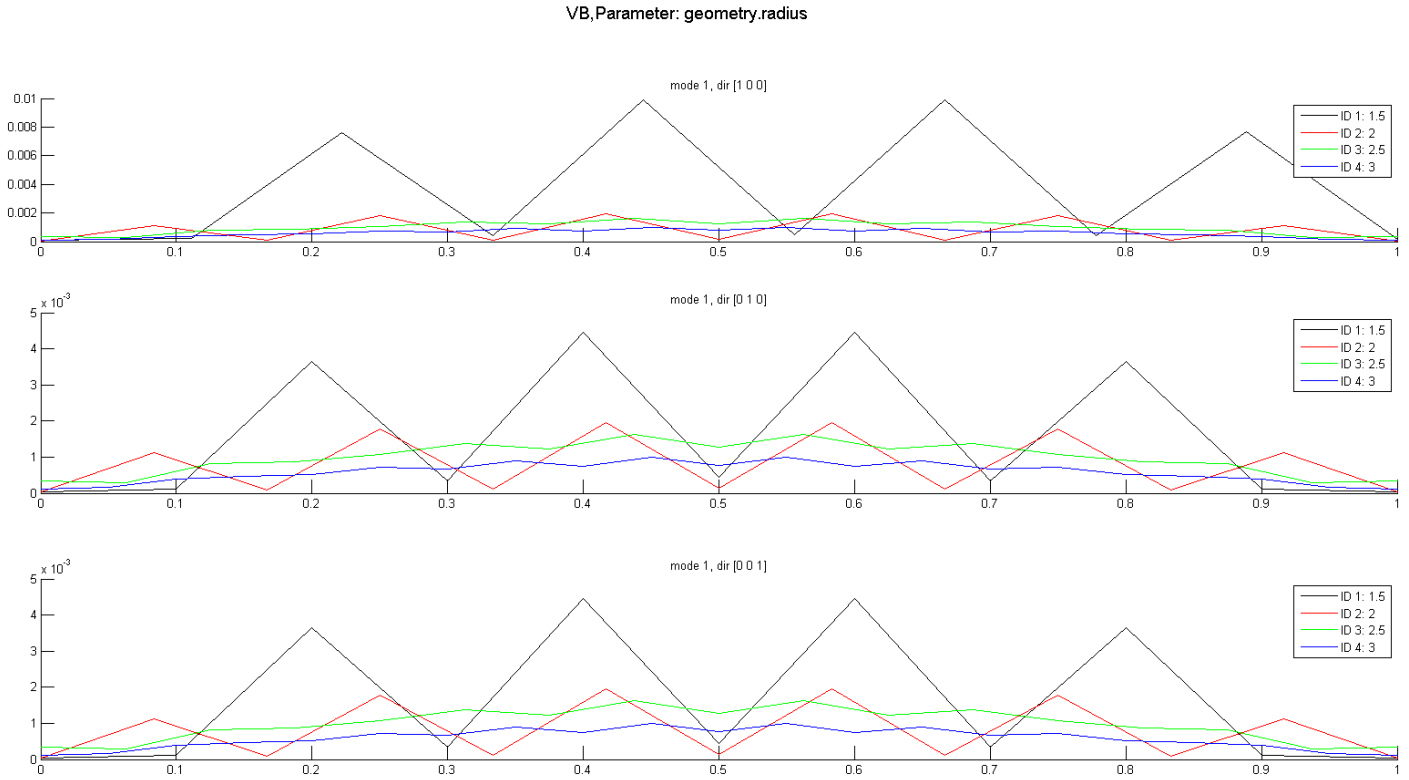

Figure 4: Wavefunctions for different radii and directions in the Valence Band Mode 1. The radii are *normalized*!

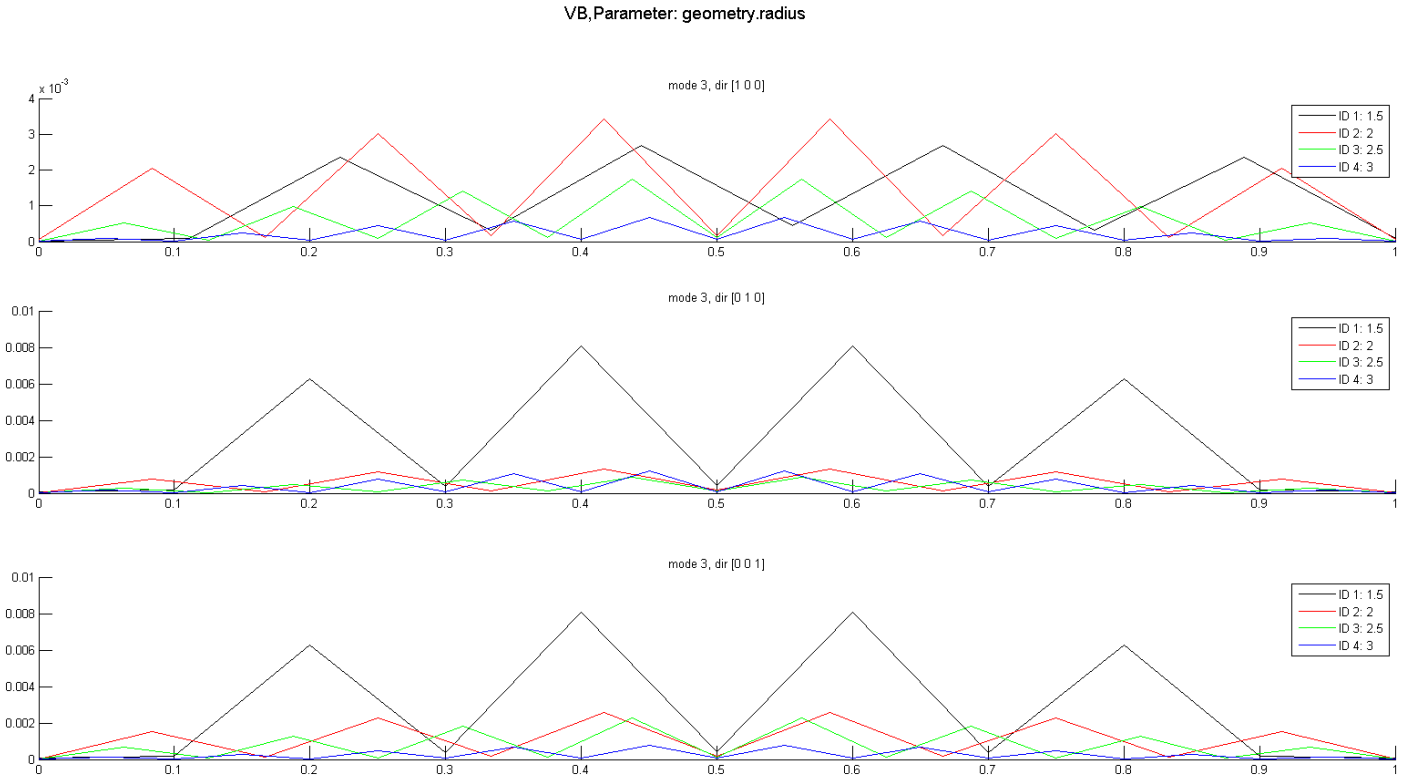

Figure 5: Wavefunctions for different radii and directions in the Valence Band Mode 3. The radii are *normalized*!

3D Wavefunctions for different Voltages

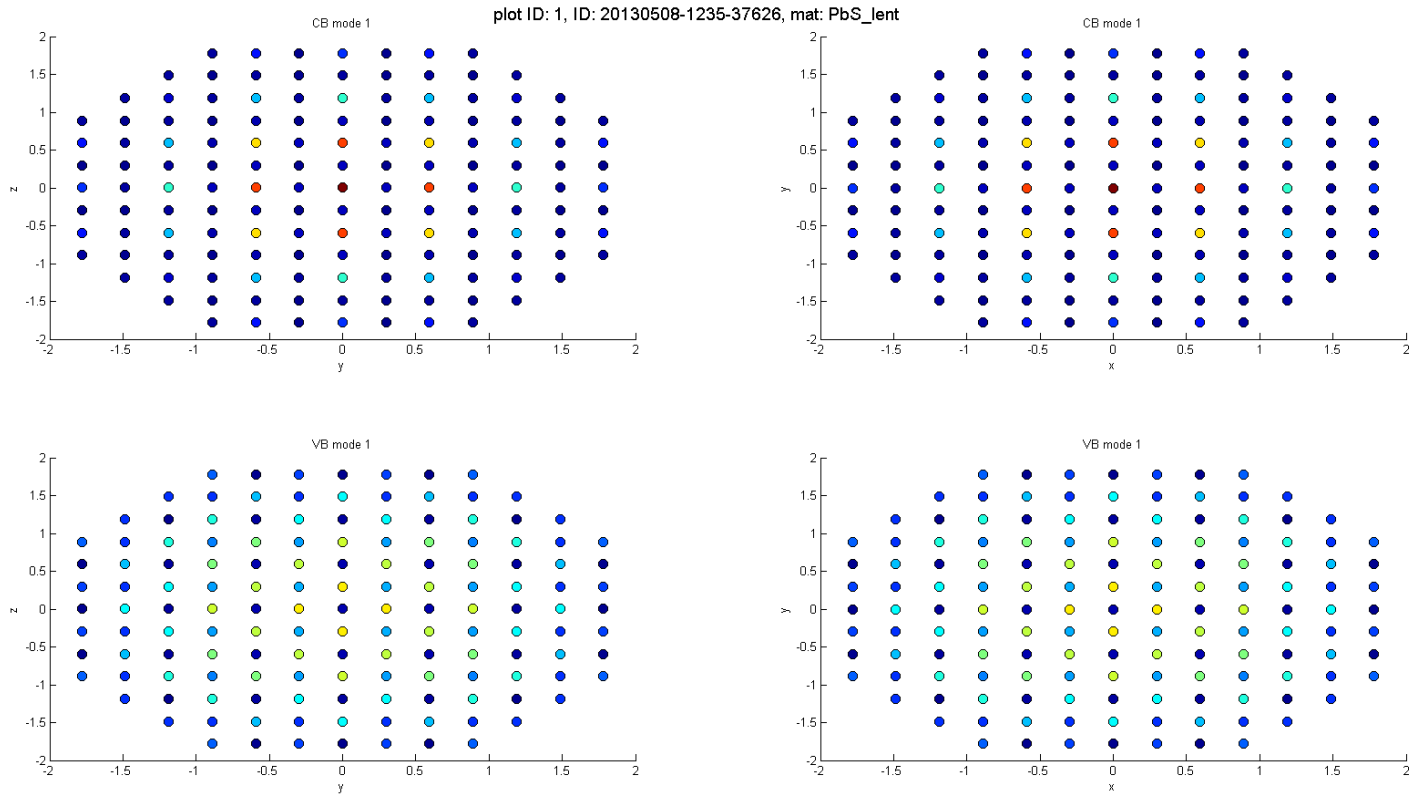

Figure 6: 3D Wavefunctions for 0V of a PbS Quantum Dot with 4 nm diameter

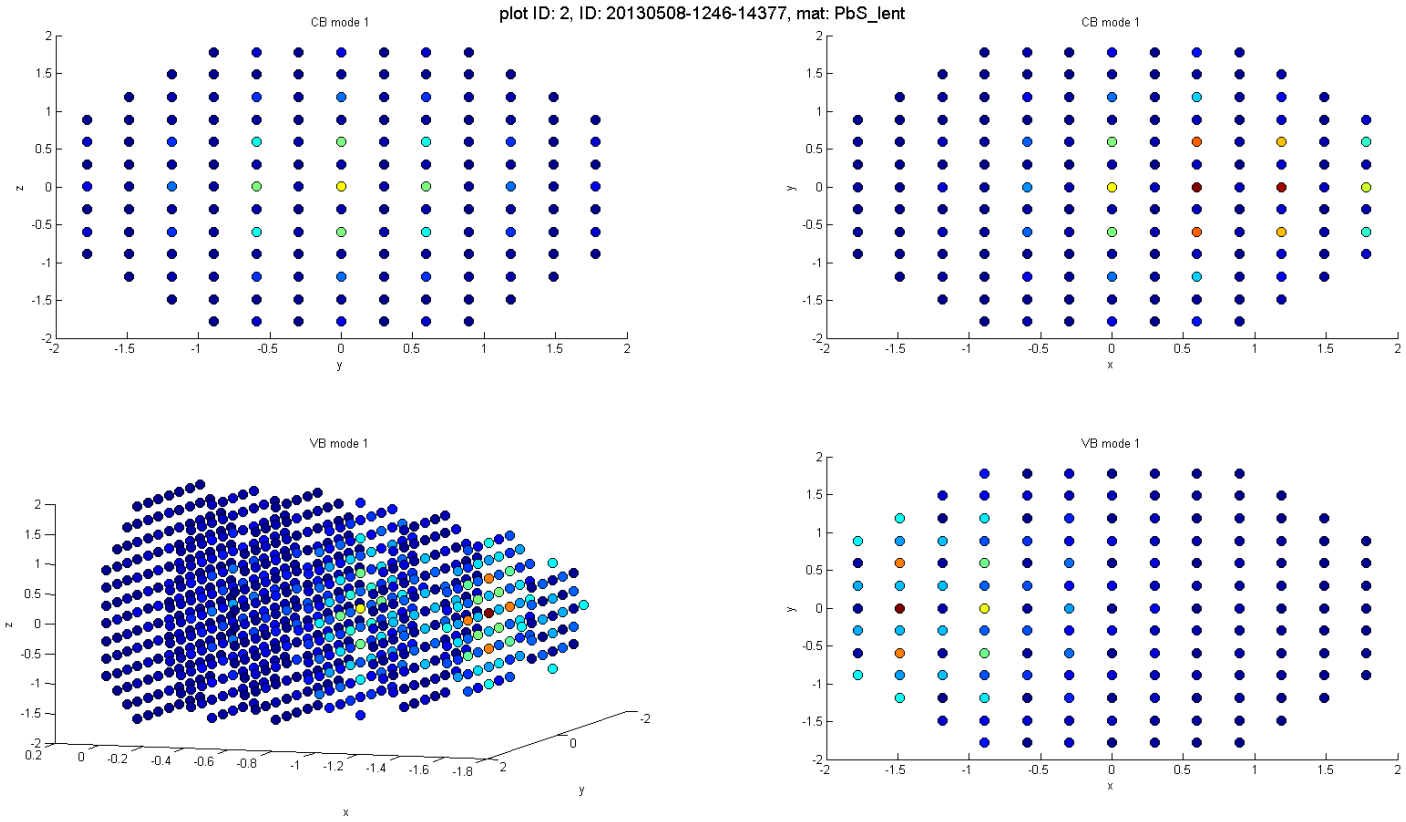

Figure 7: 3D Wavefunctions for 0.5V of a PbS Quantum Dot with 4 nm diameter

4.3 Band Gaps

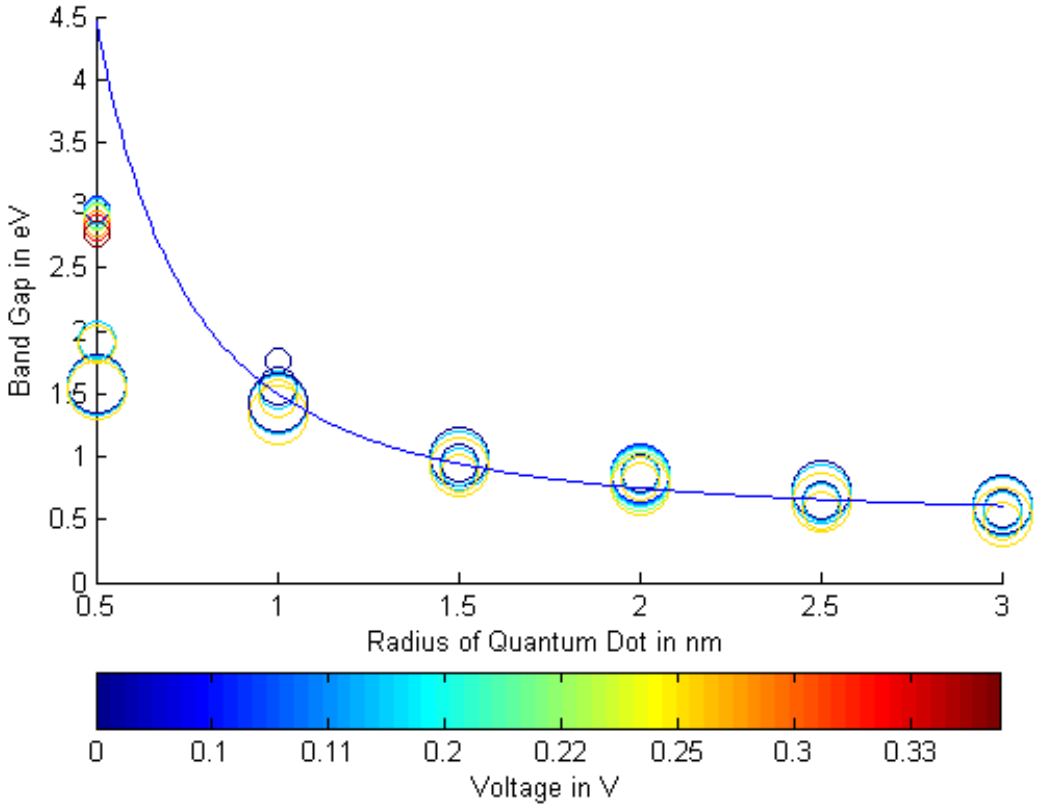

Figure 8: Plotting Band Gap against Radius of a Quantum Dot, including applied Voltage and different materials. Size of the circle indicates the material; from smallest to largest: PbSe_allan, PbSe_lent, PbS_lent. Solid blue line: $1/R^2$ dependence of the Band Gap.

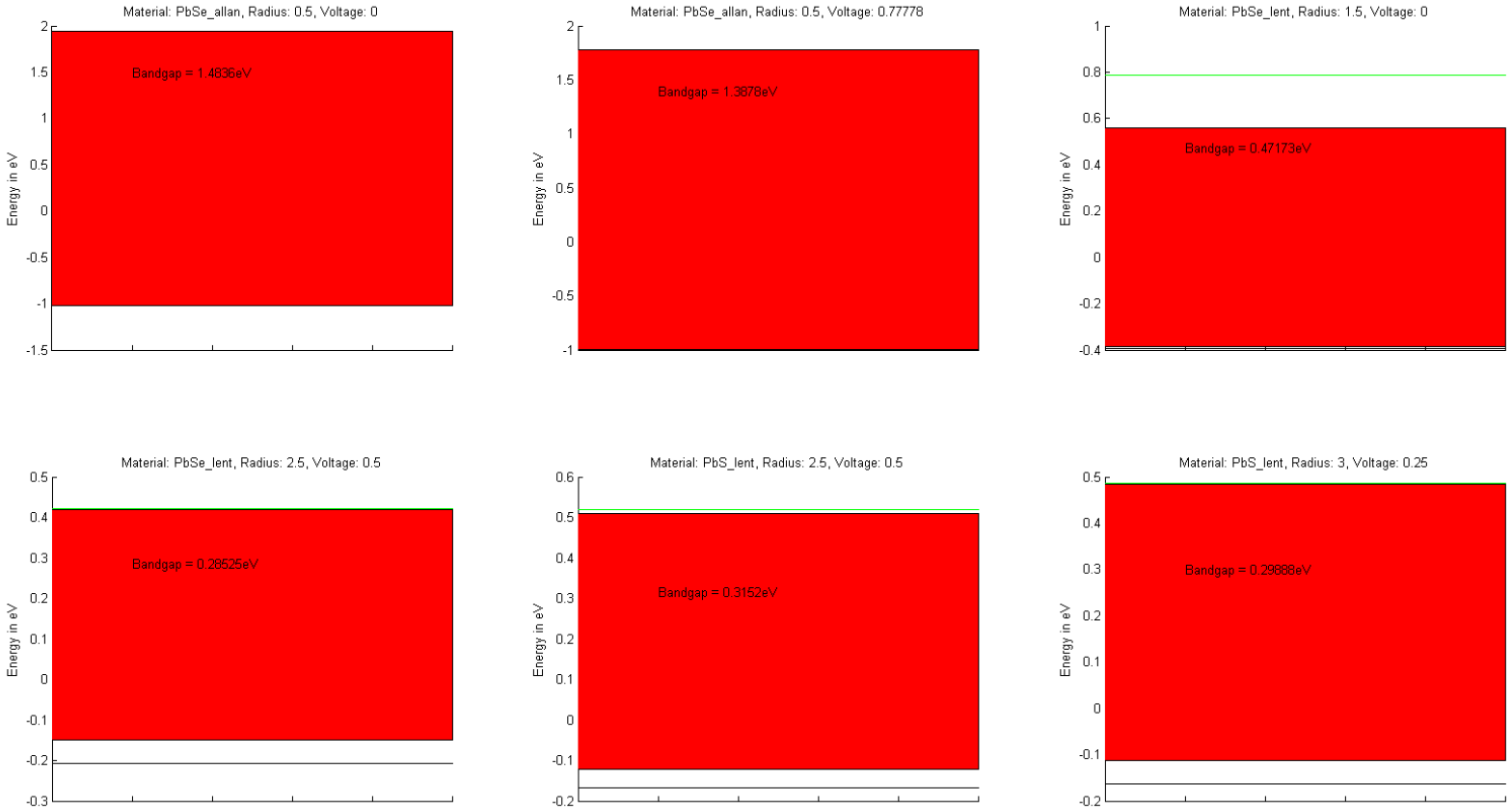

Figure 9: Green lines: Energy levels in the Conduction Band, Black lines: Energy levels in the Valence Band