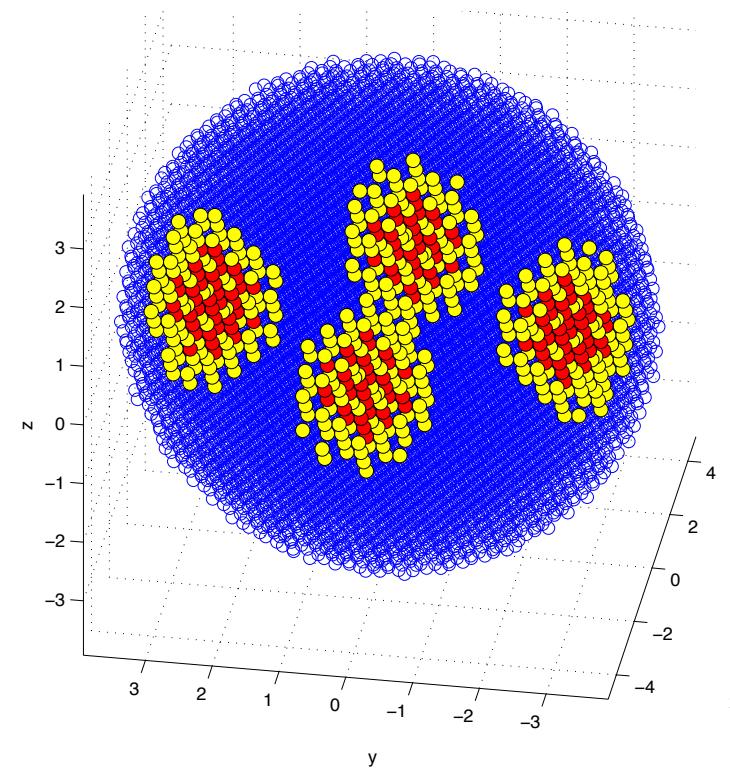


Simulation of PbS Quantum Dots

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Overview

- MATLAB Toolbox for QD-Simulations with OMEN
 - General idea
 - Demo
- PbS QD Simulations with OMEN
- Simulation Data:
 - Analysis
 - Comparison with experimental data
- Poster
- Documentation

TOM: Toolbox for OMEN in MATLAB

Simulation:

- Starting simulations intuitively and efficiently via GUI
- Automatically generate different parameter combinations

Managing the simulation data:

- Overview over previous simulations
- Filtering, deleting etc. possible

Visualisation of simulation data

- Different functions for plotting (wave functions, energy levels...)

TOM: Toolbox for OMEN in MATLAB

- Easy to use
- Well documented
- Generic and clear structure: additional functionality can easily be added (new simulation parameters, plotting functions...).
- Short Demo with some principal features

Simulation of PbS QDs with OMEN

PbS structures can now be simulated with OMEN
(Tight-binding parameters from Craig Lent-Paper)

Things to note for PbS QD simulations:

- Computing resources: PbS uses *much* more resources compared to CdS-CdSe (memory and duration). Reasons:
 - Number of orbitals (18 for PbS vs 5 for CdS-CdSe)
 - Number of modes (see below)
- More modes have to be simulated, due to high degeneracy of the energy levels.

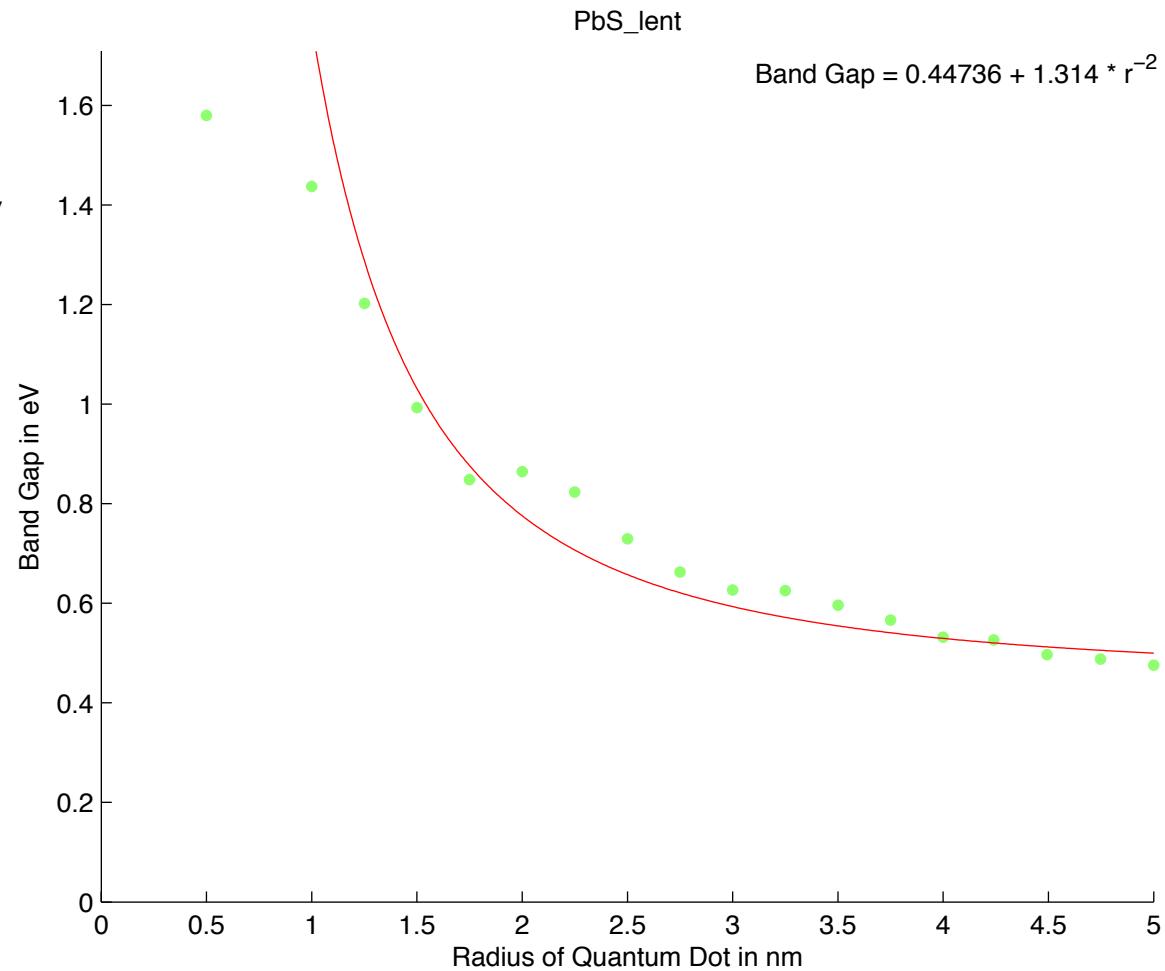
Analysis of Simulation Data

Simulated QDs:

- Radius between 0.5 and 5 nm
- Electric fields up to 2V/nm
- 20 modes for CB and VB respectively

Band gap: dependence on size of QD

- $1/r^2$ –fit: estimated bulk band gap ~ 0.42 eV:
Too big compared to the experimental value of 0.37eV
- Deviation from $1/r^2$ dependence for small QDs



Band gap: comparison with experimental data

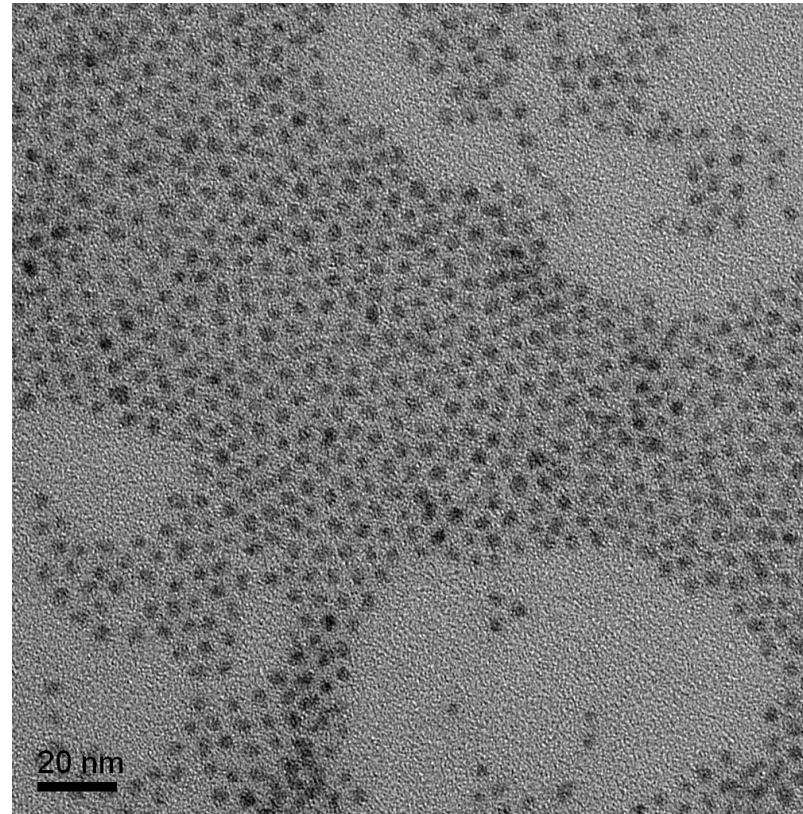
Generally: Correct tendency, but simulated band gap much smaller than suggested by absorption spectra of PbS QDs. Possible reasons:

- Real QDs are not perfect: impurities, non uniform size ...
- Simulation parameters
- Size: correctly determined the size from TEM images? (see next slide)

	Experimental ϕ - Simulated ϕ			
	$\sim 2.97\text{nm} - 3\text{nm}$ PbS - 261 ¹	$\sim 3.21\text{nm} - 3\text{nm}$ PbS - 61	$\sim 3.95\text{nm} - 4\text{nm}$ PbS - 190	$\sim 4.97\text{nm} - 5\text{nm}$ PbS - 220
Energy at PL peak	1.4529eV (853nm)	1.2256eV (1012nm)	n/a	1.0040eV (1235nm)
Band gap experimental	1.7487eV (709nm)	1.5194eV (816nm)	1.2808eV (968nm)	1.0489eV (1182nm)
Band gap simulated	0.9929eV	0.9929eV	0.8645eV	0.7296eV

Band gap: comparison with experimental data

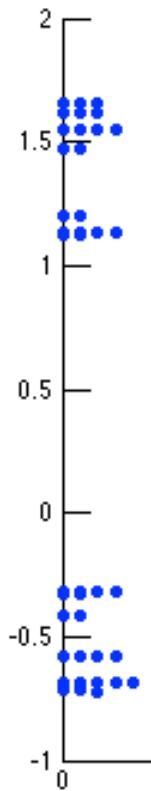
Possible issue: The size of the QDs is difficult to determine...



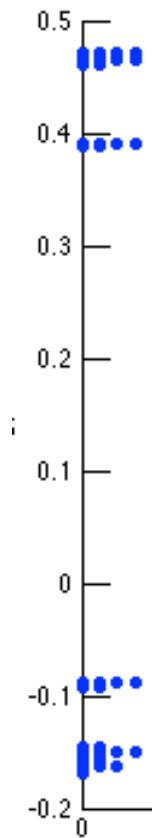
Energy levels for PbS QDs

Band edges: 8 quasi degenerate energy levels.

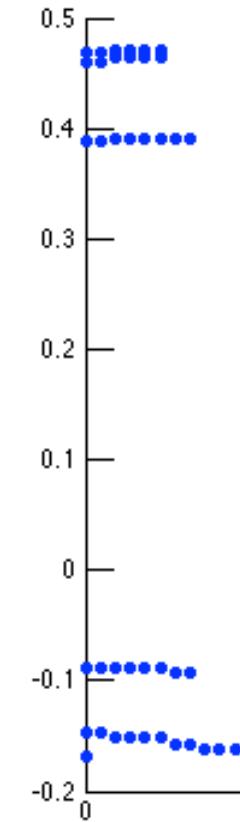
2nm QD



10nm QD



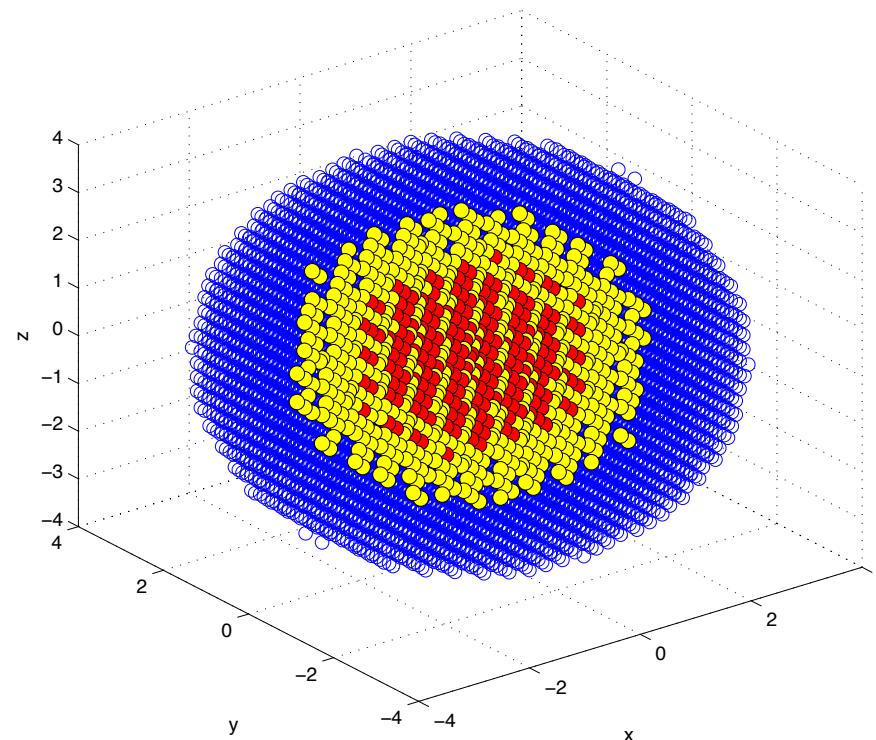
10nm QD, better visibility for (quasi) degenerate states.



Wave functions for band edge states, big QDs

Spherical shape: „1S orbitals“

plotID: 1, mat: PbS_lent, Efield: 0, ModNr: 6, E-Level: 0.437598 eV

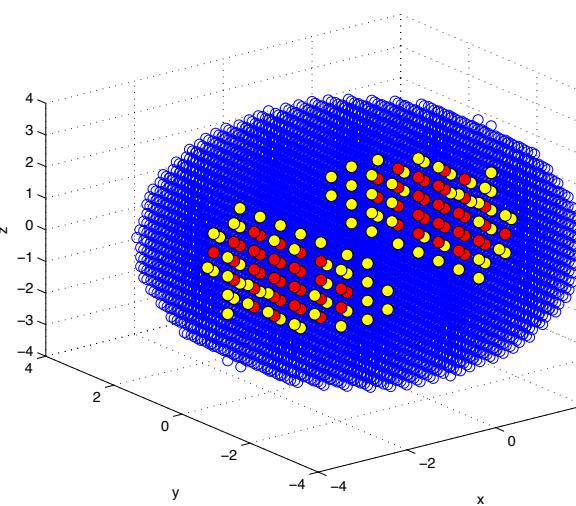


Probability density for a CB state near band edge, of a 8nm QD.

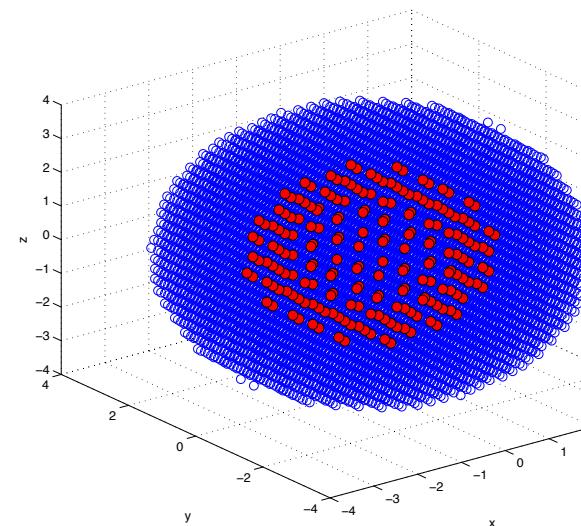
Wave functions for higher modes

Non spherical shapes: Probability density for CB modes 10, 14, 20.

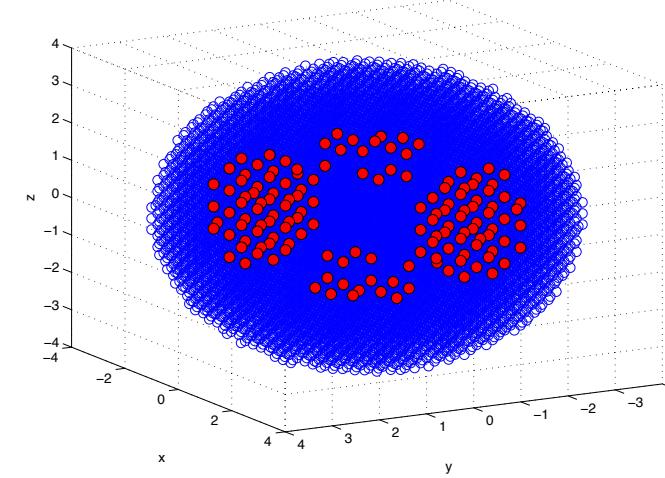
plotID: 1, mat: PbS_lent, Efield: 0, ModNr: 10, E-Level: 0.52



plotID: 1, mat: PbS_lent, Efield: 0, ModNr: 14, E-Level: 0.532099 eV

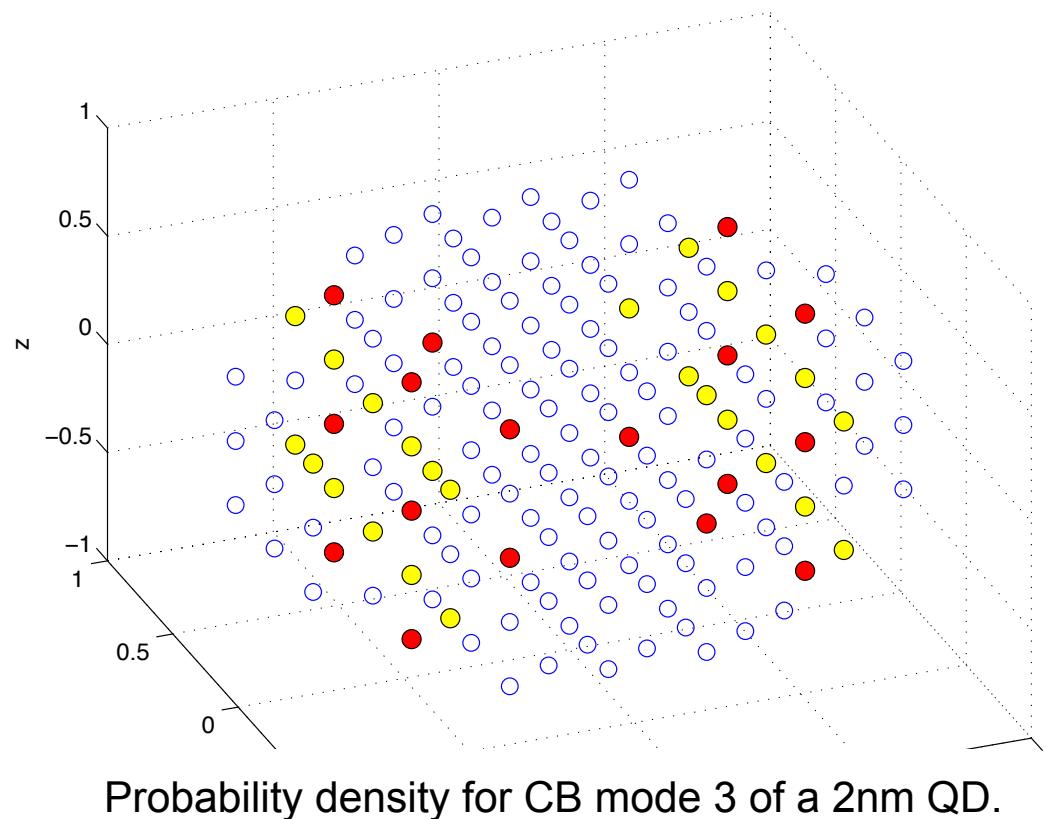


plotID: 1, mat: PbS_lent, Efield: 0, ModNr: 20, E-Level: 0.547438 eV



Wave functions for small QDs

Near band edge states: spherical symmetry of wave fn is lost for some states.
Close to reality?

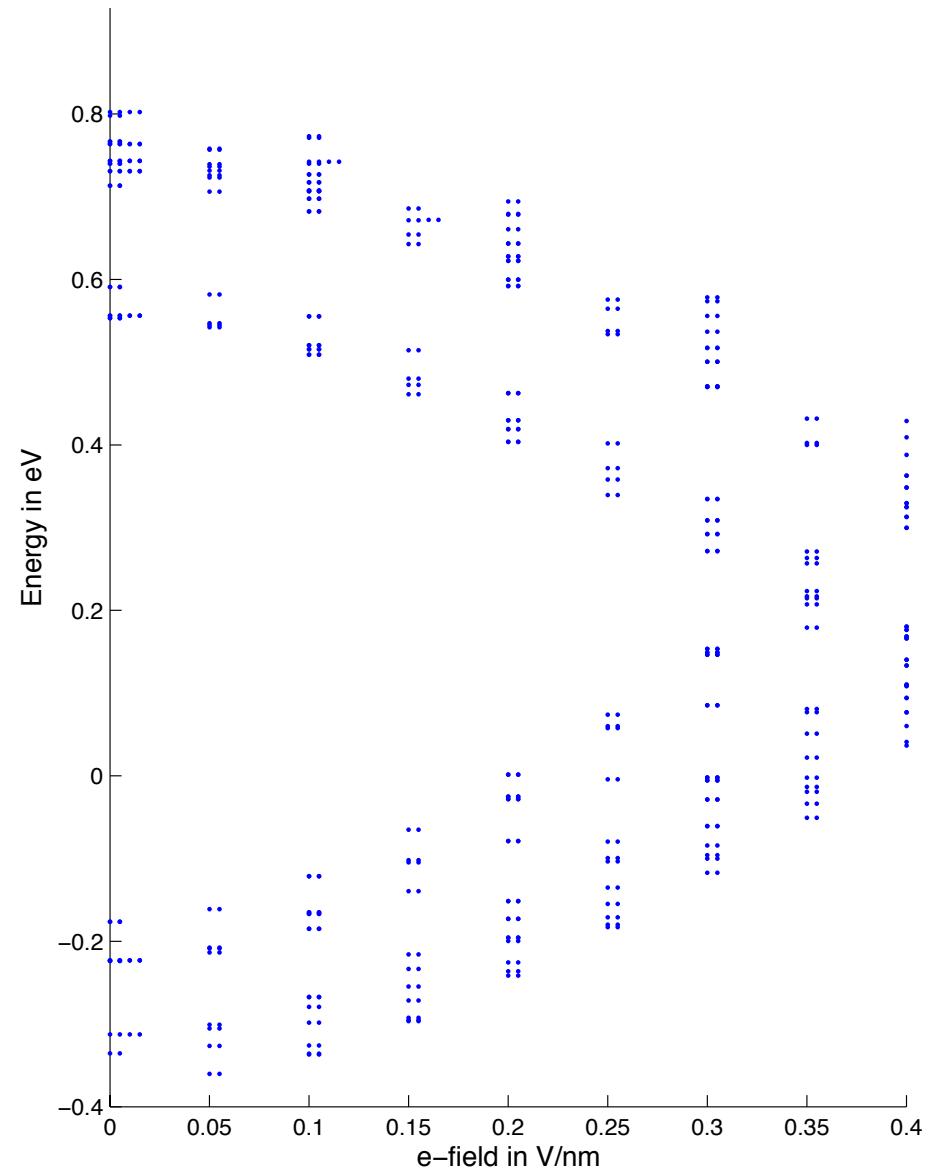


Energy levels and electric field

Energy levels for a 5nm QD plotted against applied electric field.

Band gap gets smaller for higher fields.

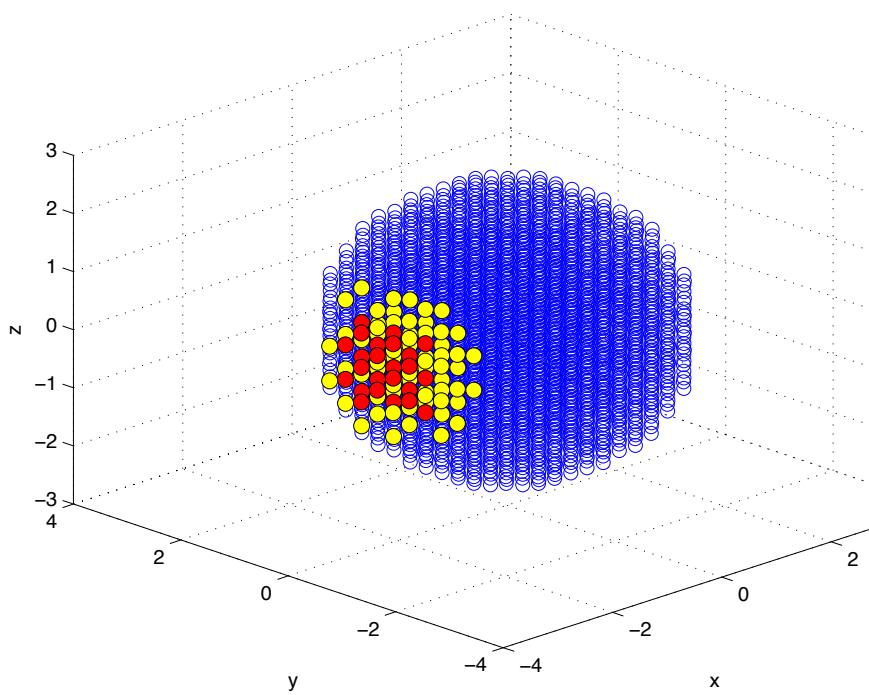
8-fold degeneracy of band edge states is lost (twofold degenerate states remain).



Wave functions and electric field

Shift of wavefunction, depending on hole-like resp. electron-like character, to the left or right.

plotID: 1, mat: PbS_lent, Efield: 0.2, ModNr: 10, E-Level: -0.028155



plotID: 1, mat: PbS_lent, Efield: 0.2, ModNr: 19, E-Level: 0.429667 eV

