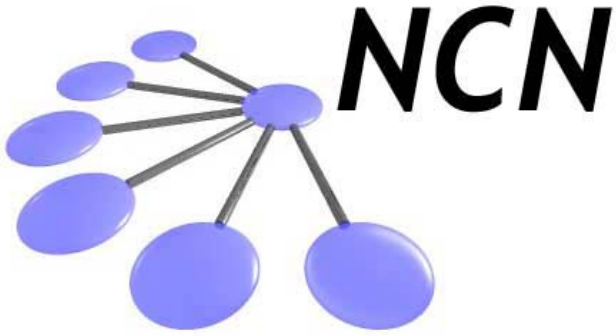
Long-Range Strain in InGaAs Quantum Dots



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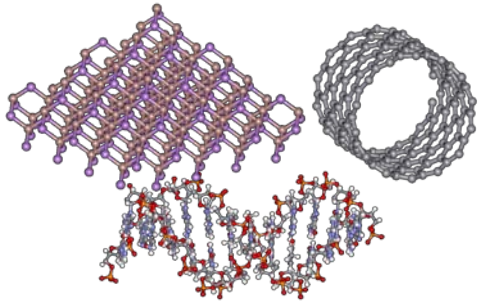
Atomistic strain calculation followed by sp3s*d5 tight binding eigenvalue solution



Structure

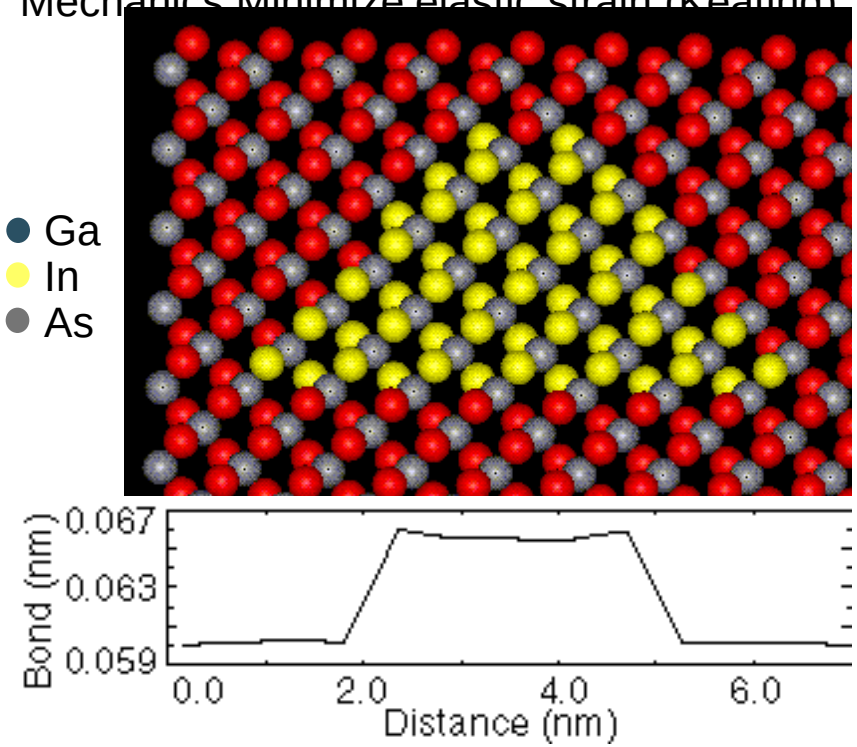
Dot Formation Due to Strain:

- Self-Assembly induced by strain in GaAs/InAs and Si/Ge material systems.
- Bond length and orientation distortion

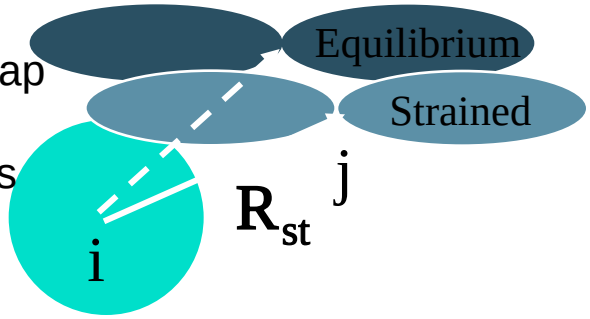
Strain affects Electronic Structure:

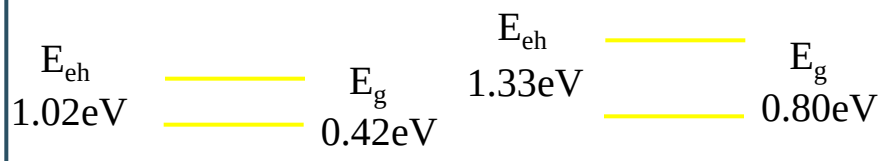
- Tight binding models can predict this!

Mechanics:Minimize elastic strain (Keating)



Electronics:
Orbital overlap changes
=> bandgaps and masses





Unstrained Dot Strained Dot

Pyramidal InAs Dot Simulation

Base: 7nmx7nm Height: 3nm Embedded in GaAs

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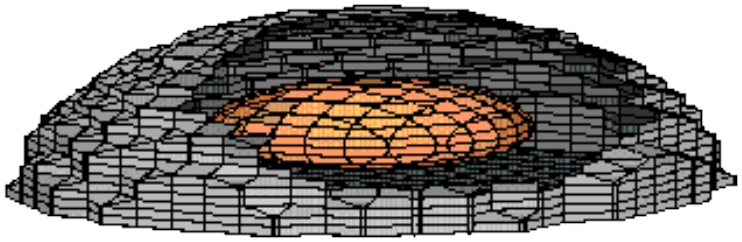
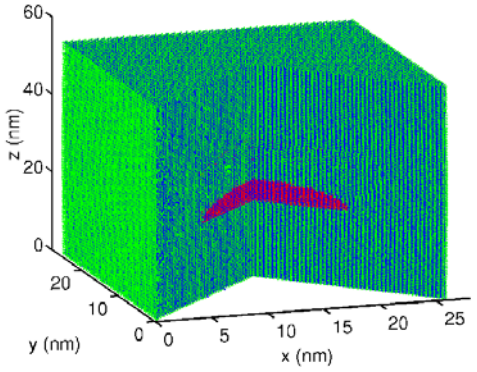
Quantum dot:
30nm diameter
5nm height

Embedded in
GaAs

Eigenenergy = X eV
Eigenstate





Physical Structure:
Ordered Crystal

Relax the Strain:
Move Atoms Slightly

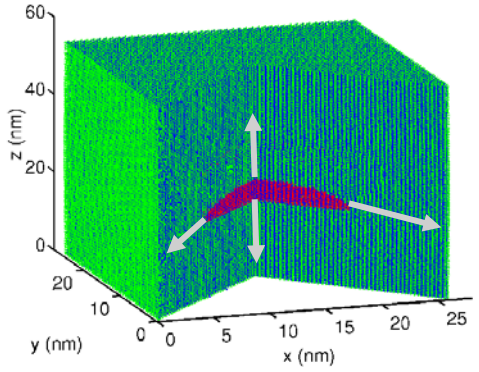
Calculate Electronic
Structure for Fixed Atoms

How do the Eigenenergies depend on the GaAs Buffer Size?

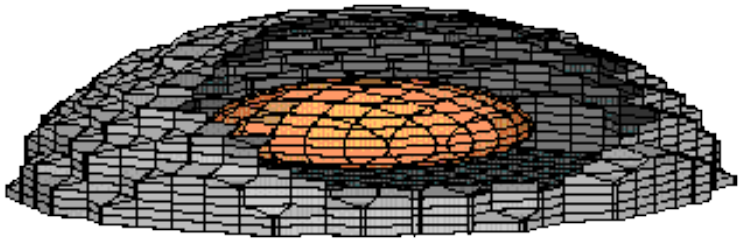
Quantum dot:
30nm diameter
5nm height

Embedded in GaAs

Free strain BC



Eigenenergy = X eV
Eigenstate

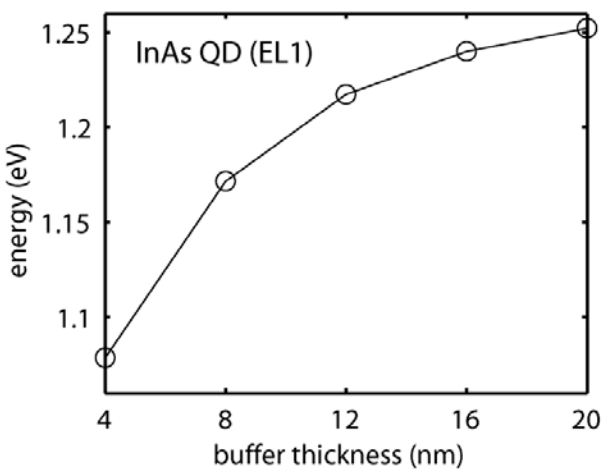


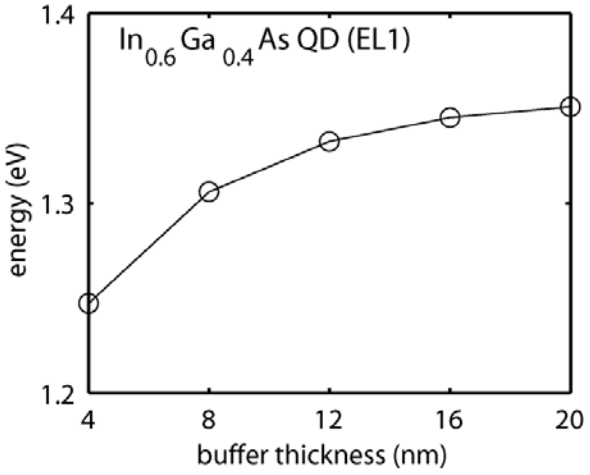
Physical Structure: Ordered Crystal

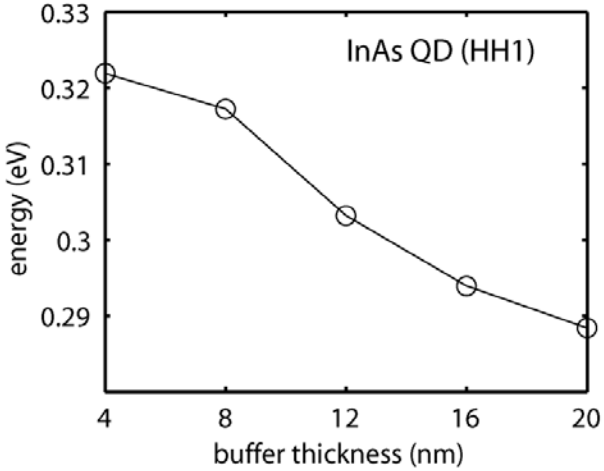
Relax the Strain: Move Atoms Slightly

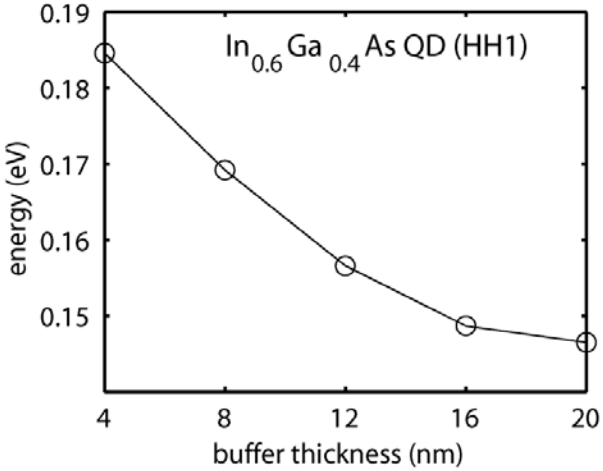
Calculate Electronic Structure for Fixed Atoms

Ground State Energy Dependence on Buffer Size



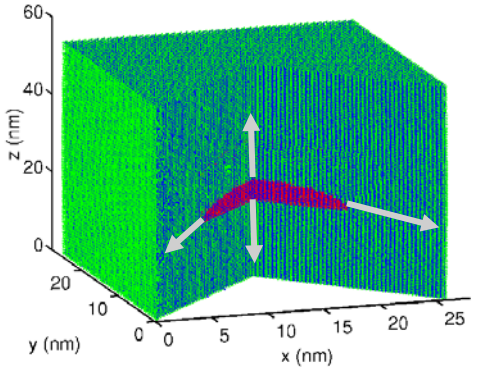






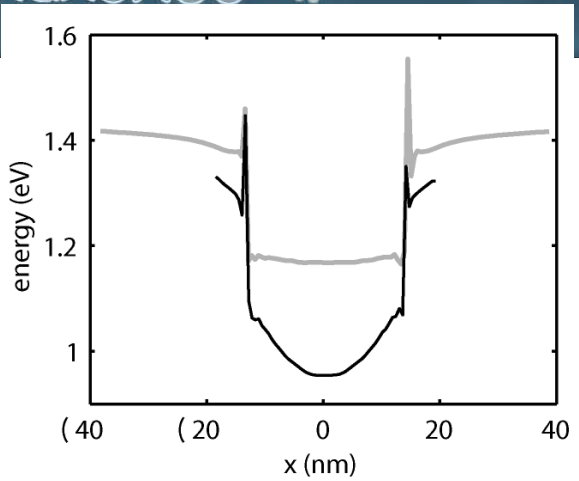
Quantum dot:
30nm diameter
5nm height

Vary GaAs buffer from 4nm to 20nm in all directions
Free BC on atoms
Closed BC on electrons

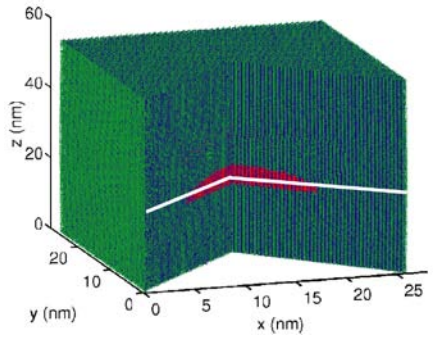


- Electron and hole ground states depend strongly on the GaAs buffer size
- Dependence is weaker for the electron states in the alloyed dot.

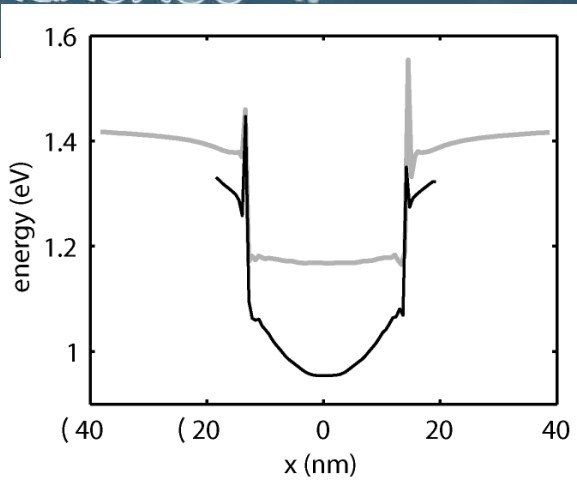
Strain Effects on Local Band Structure

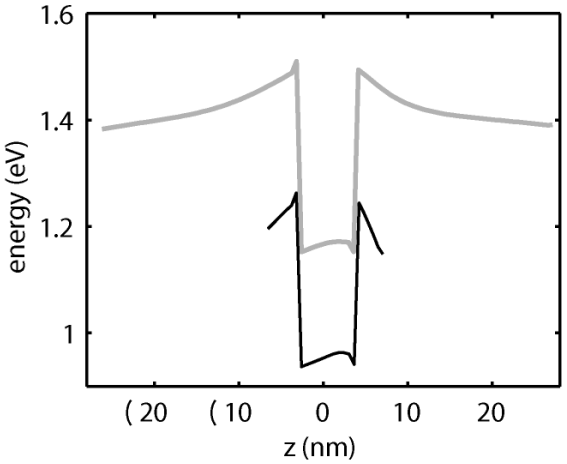


- Strain shows a long-range effect
- Electron confinement in x changes shape

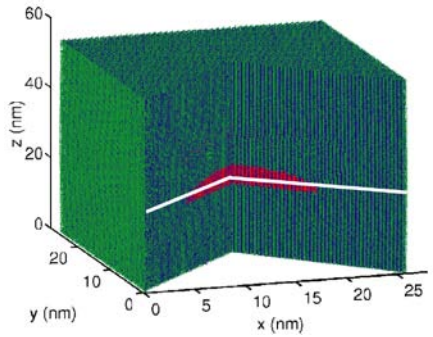


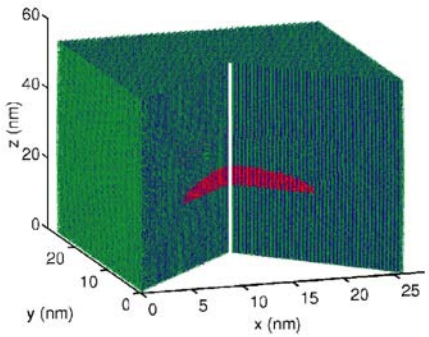
Strain Effects on Local Band Structure



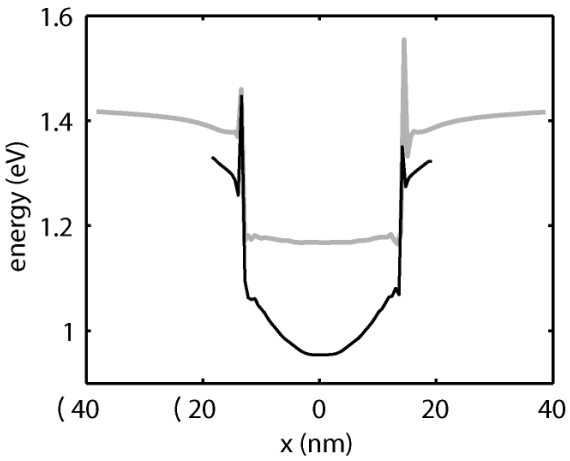


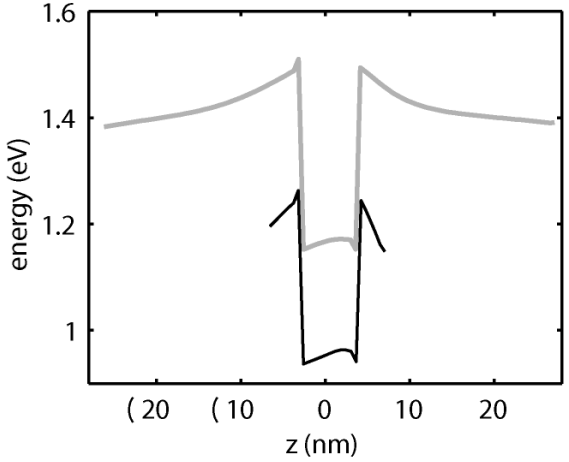
- Strain shows a long-range effect
- Electron confinement in x changes shape
- Electron confinement in z shows vertical shift

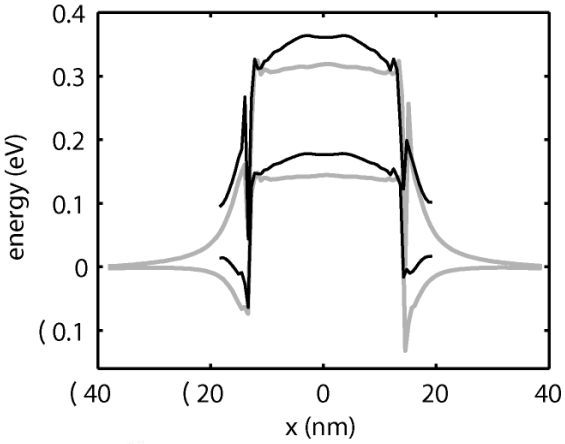


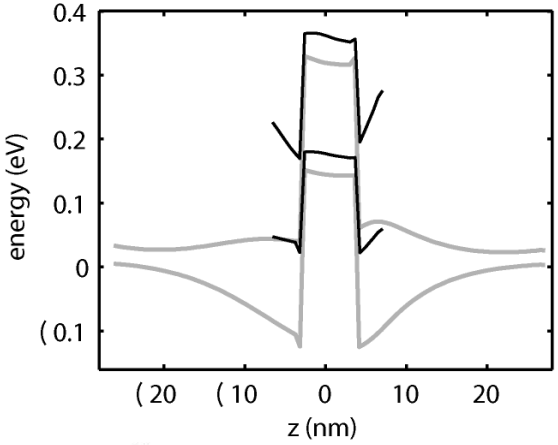


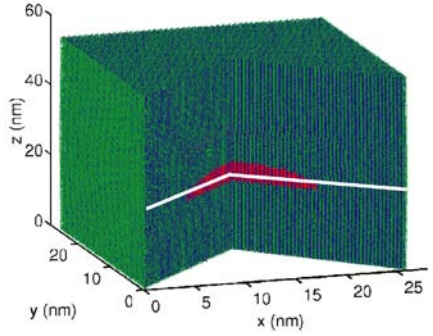
Strain Effects on Local Band Structure

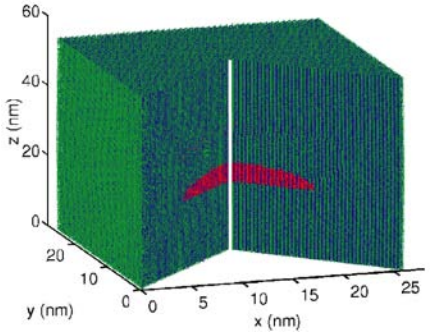






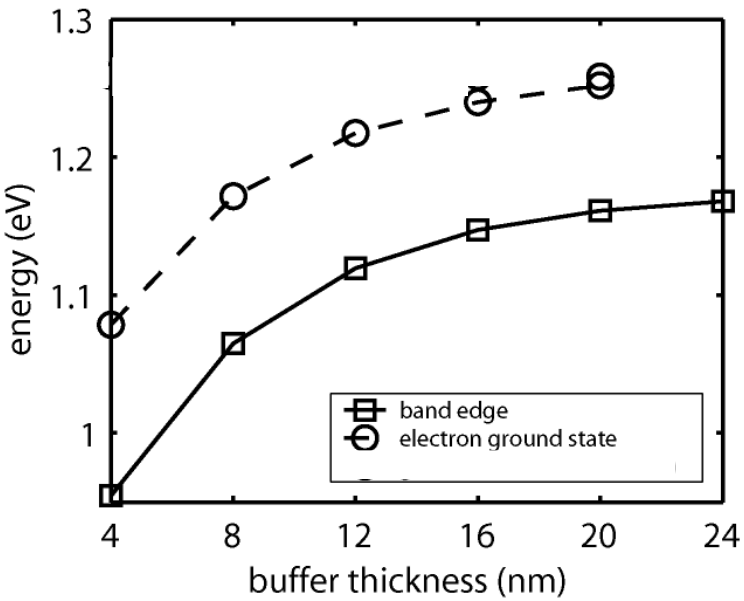






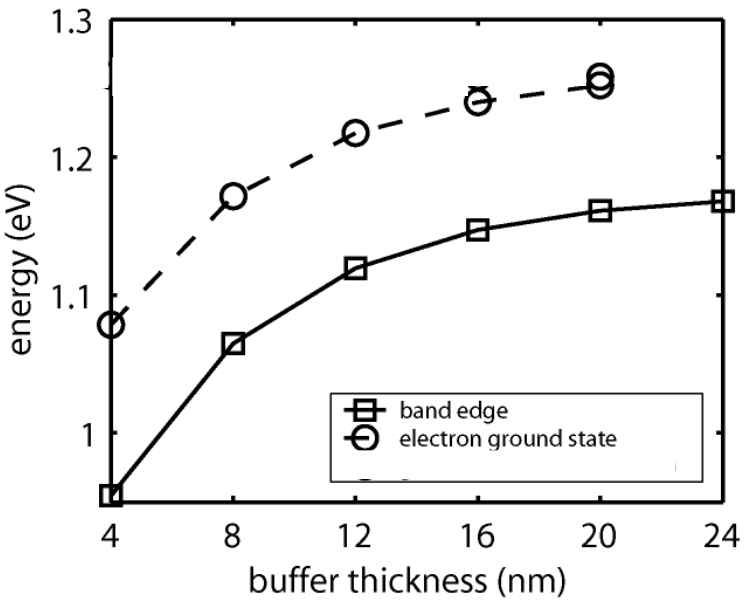
- Strain shows a long-range effect
- Electron confinement in x changes shape
- Electron confinement in z shows vertical shift
- Hole confinement in x small modulations
- Hole confinements in z vertical shift, no convergence yet!

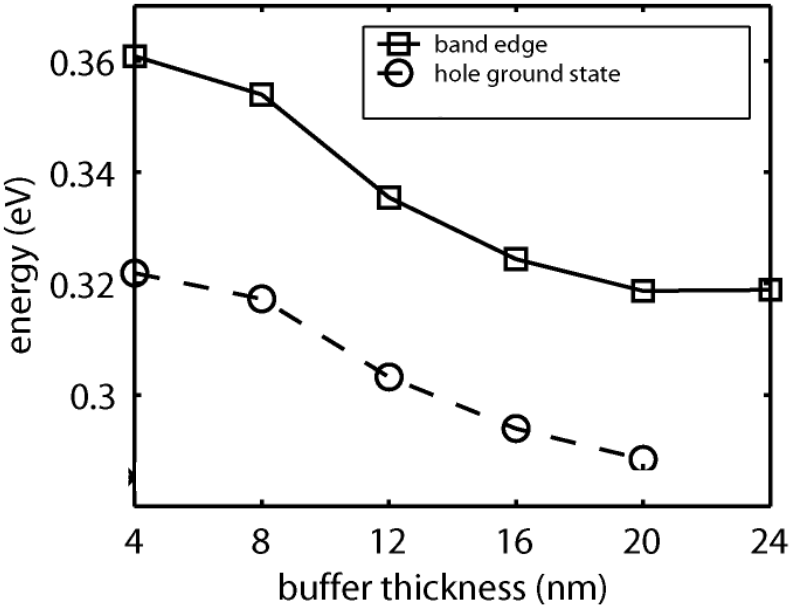
Bandedges and Eigenstates



- Electron ground state follows the bottom of the conduction band closely

Bandedges and Eigenstates

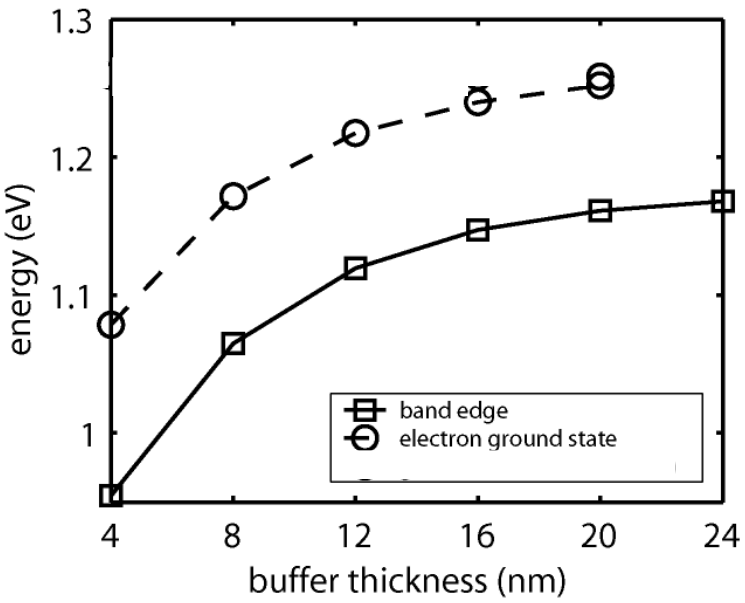


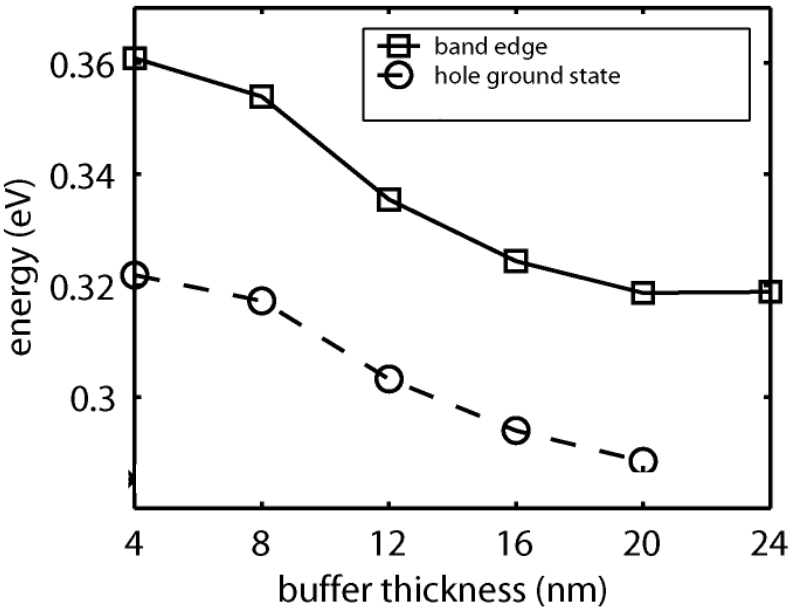


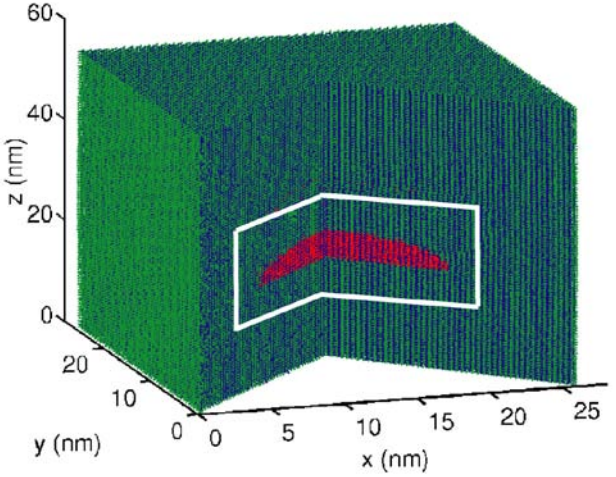
- Electron ground state follows the bottom of the conduction band closely

Valence ground state follows the top of the valence band closely

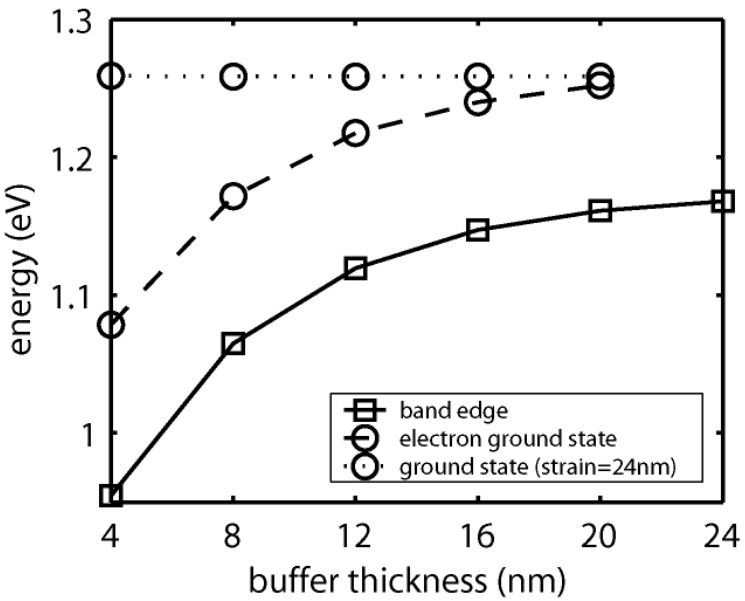
Decoupled Strain and Electronic Boundary Conditions

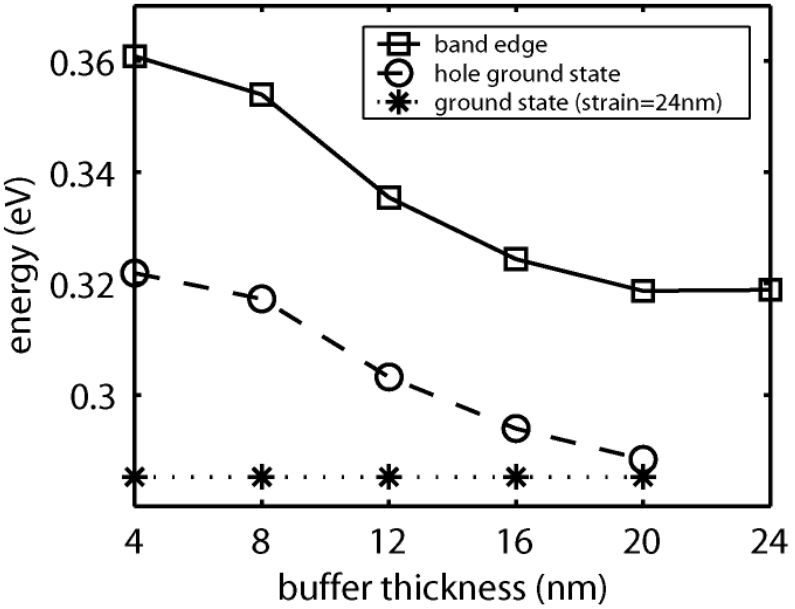




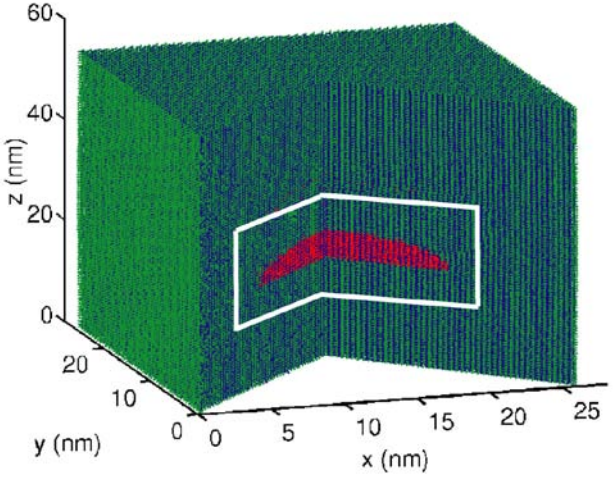


Decoupled Strain and Electronic Boundary Conditions





- Compute strain in 24nm buffer system (9 million atoms)
- Vary size of the electronic system buffer
  => Electronic states virtually unaffected

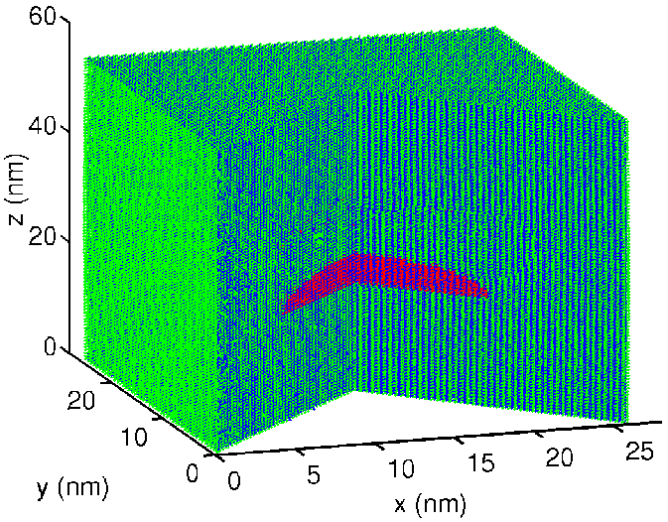


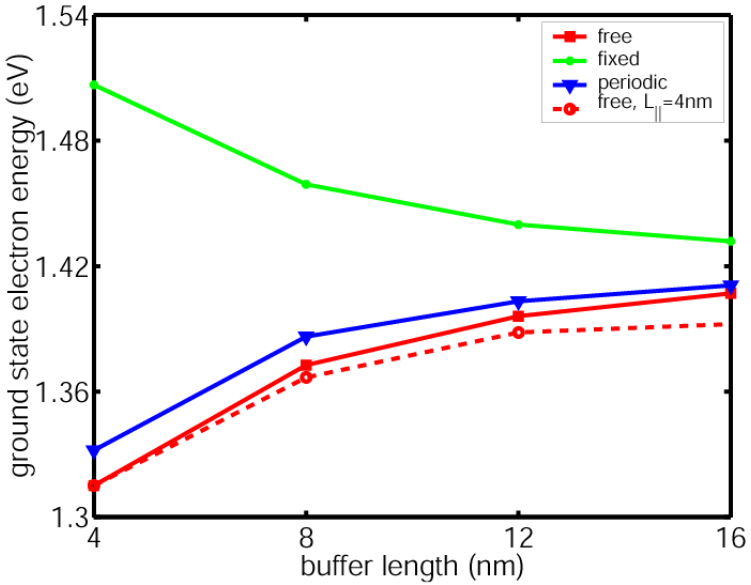
- Hard-wall electronic boundary conditions have little effects.
- Long-range strain effects dominate the quantum dot states.
- Neighboring dots will have strong effects!

Issues with Boundary Conditions / System Size

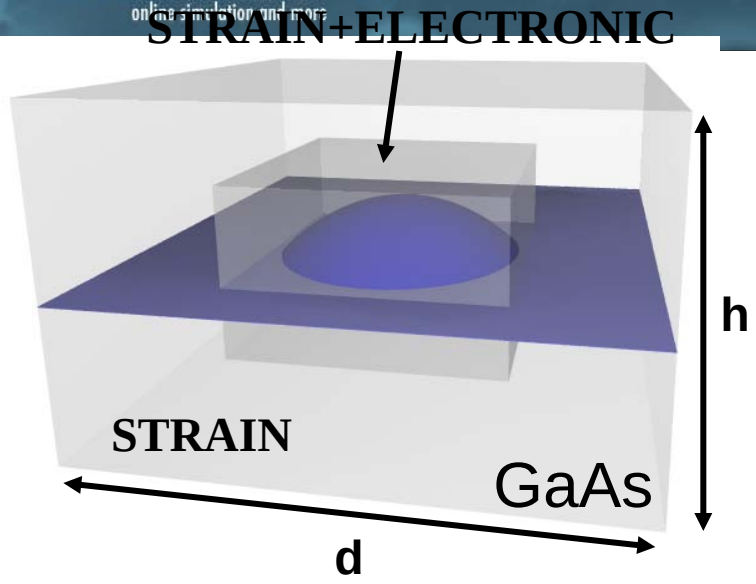
Effect on ground state electron energy:

- System: Dome-shaped $In_{0.6}Ga_{0.4}As$ QD 15nm radius; 5.4 nm height
- *Free BC*: no constraints on QD; strain and ground state energy are underestimated
- *Fixed BC*: QD boundary pinned; strain and ground state energy are overestimated
- **Periodic** BC ($k_{supercell}$=0): Eigenvalues lie in between free and fixed case, but results are much closer to case of free BC.





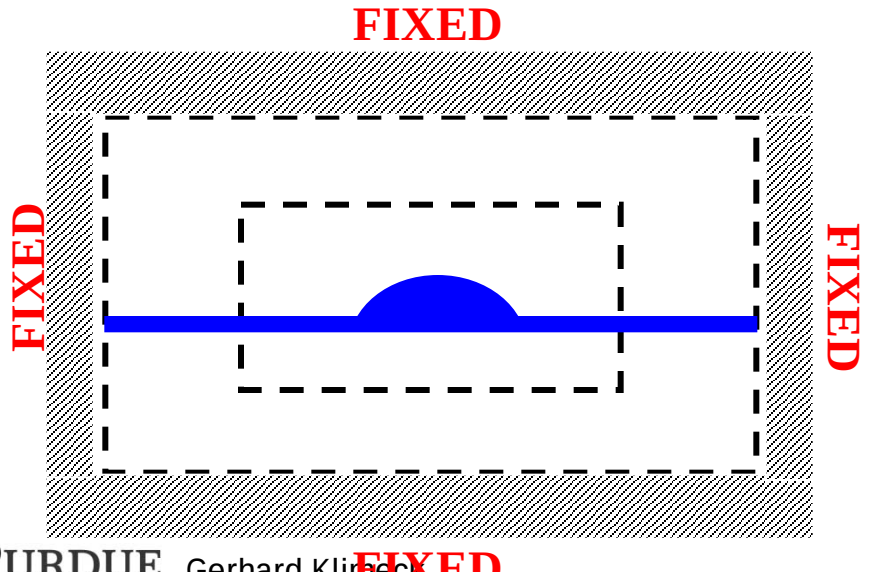
sp3d5s* Approach – test system



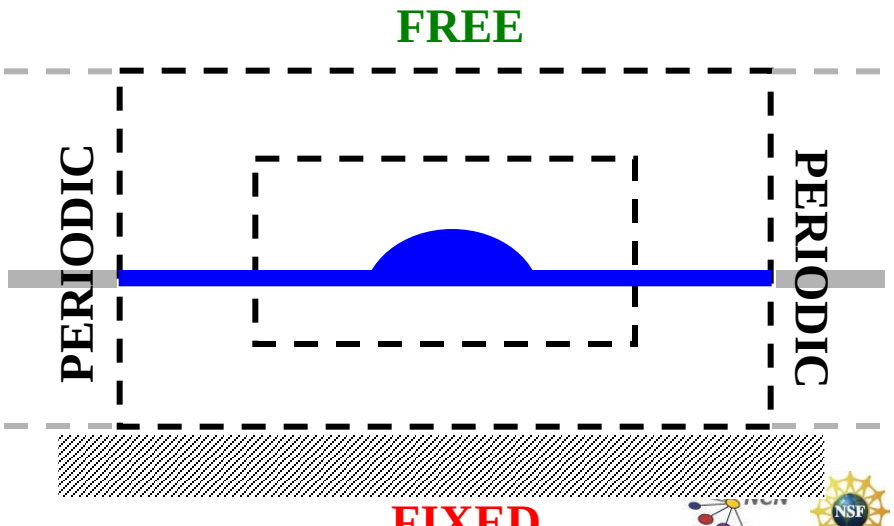
Dome-shaped InAs QDOT:

Diameter 18.1 nm, Height 1.7nm
W thickness: 0.6 nm

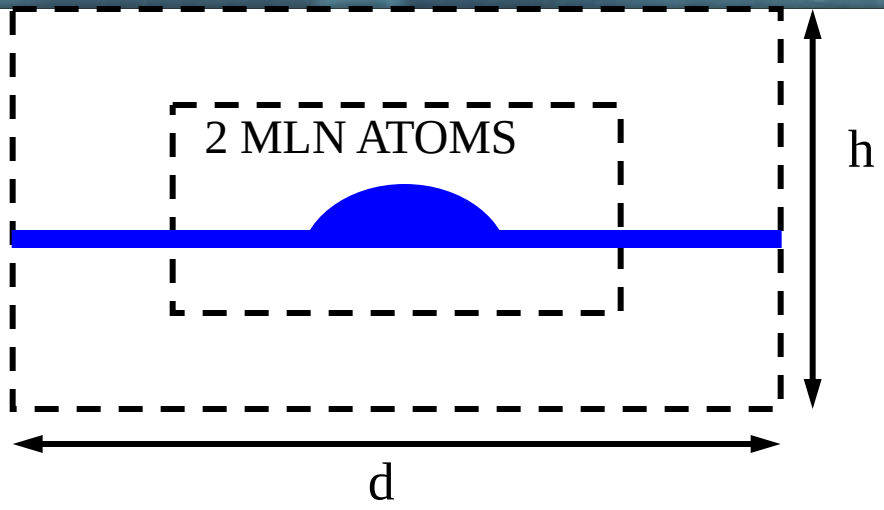
DEEPLY BURIED SINGLE QD

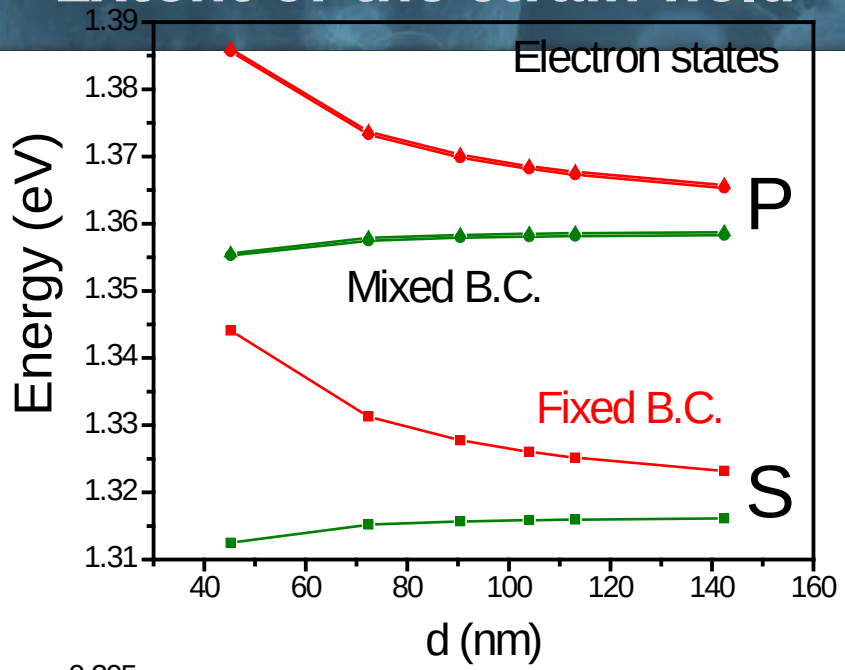


ARRAY OF QDs WITH FINITE CAP

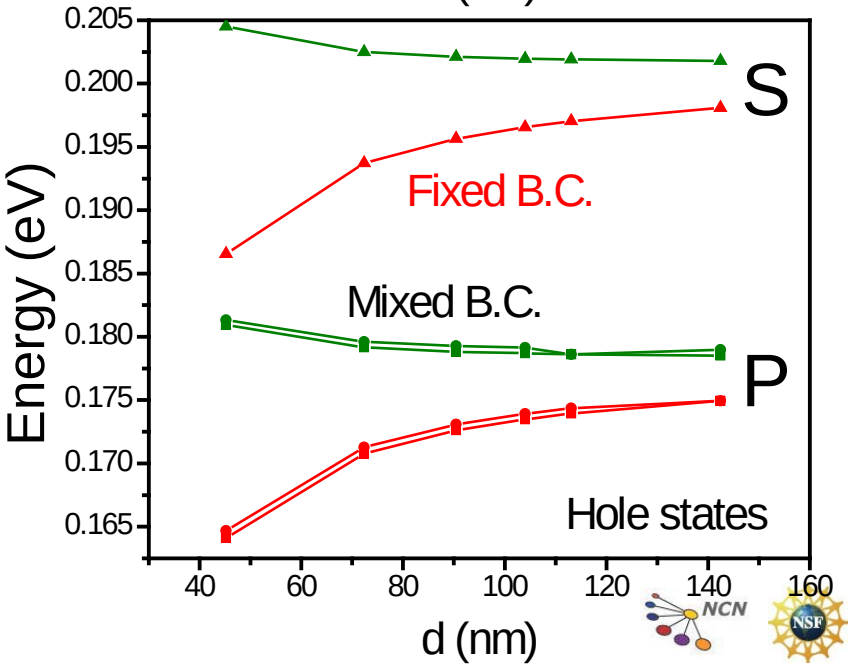


Extent of the strain field



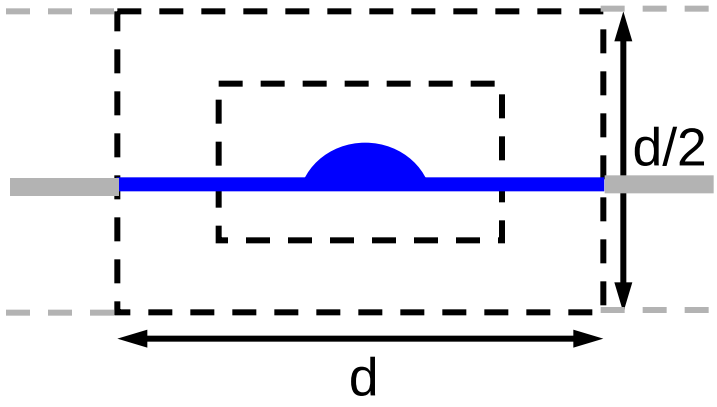


- **Ratio *d/h* Is fixed to 2**
- **Electronic domain - 2 Mln atoms**
- **Strain domain - up to 64 mln at.**
- **Computations for the**
  Deeply buried dot and
  The dot array with free surface

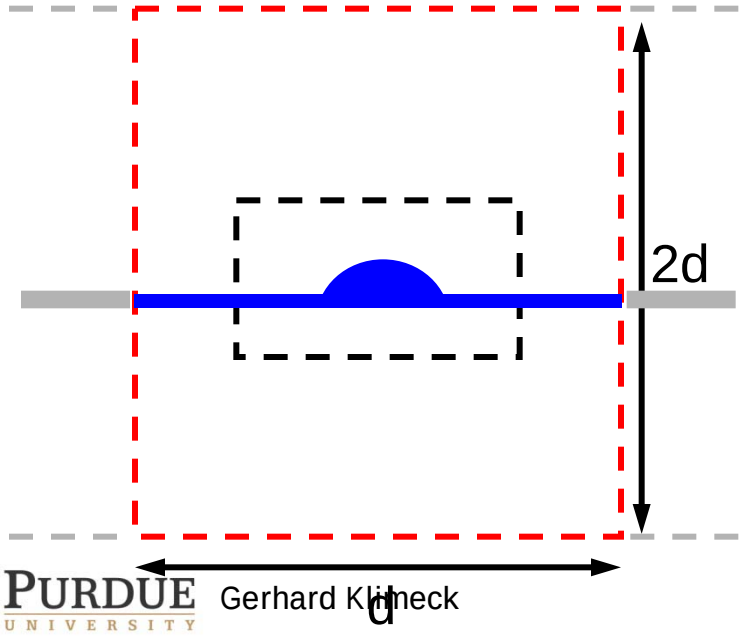


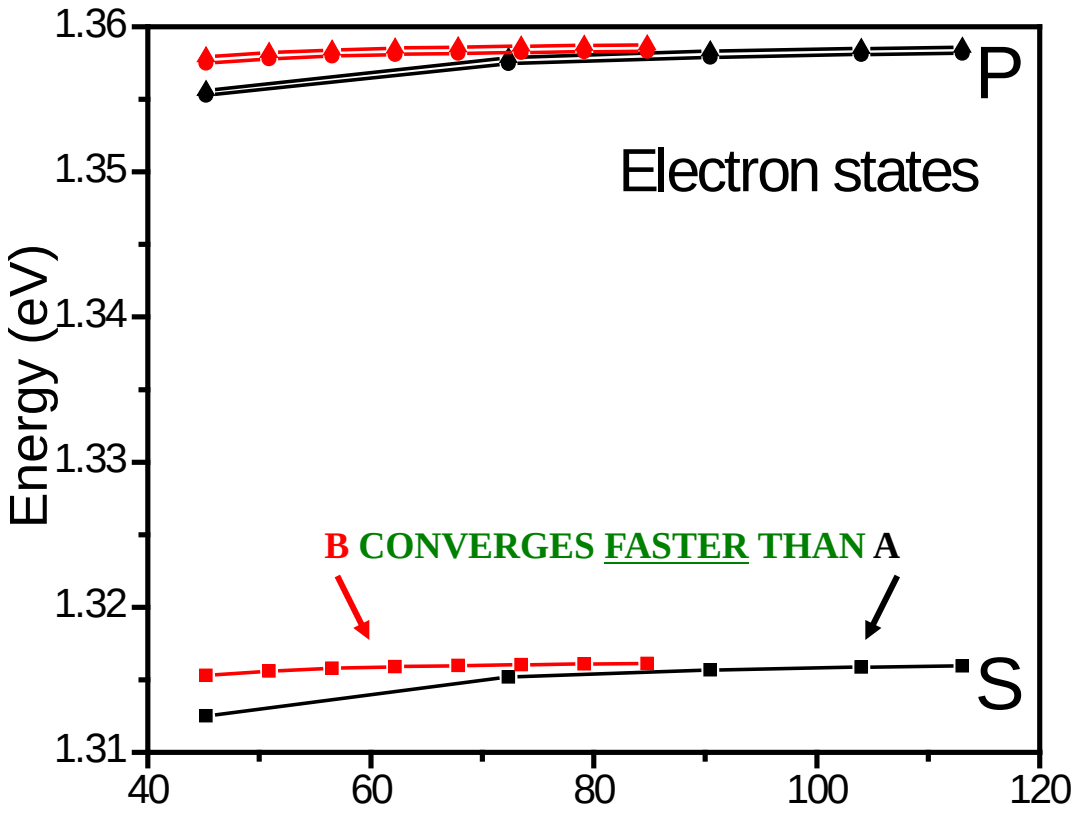
Directionality of the strain field

A) laterally oriented Strain domain:

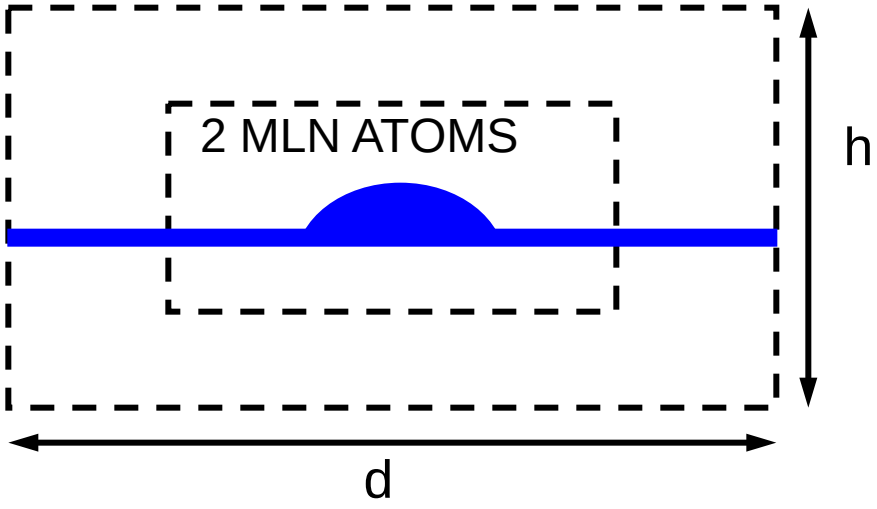


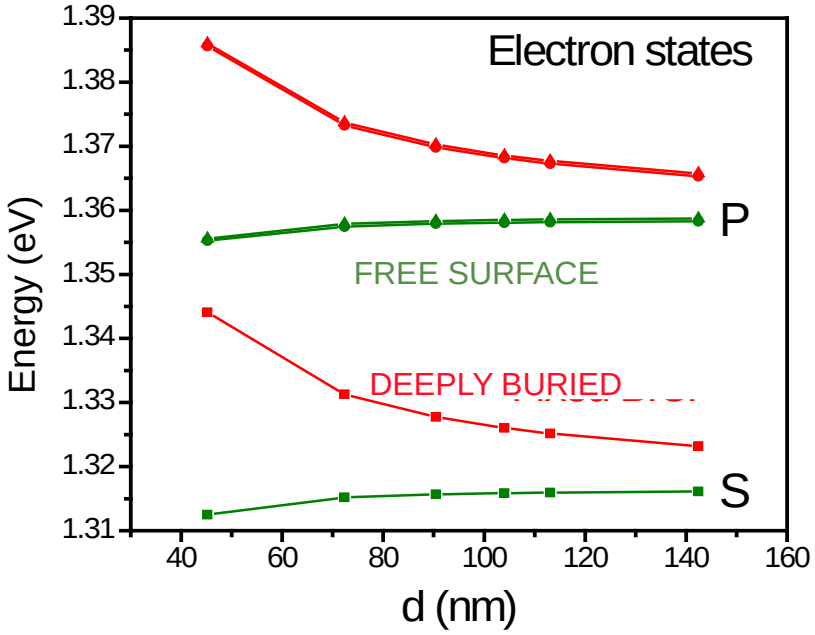
B) Vertically ORIENTED STRAIN DOMAIN:





Extent of the Strain Field





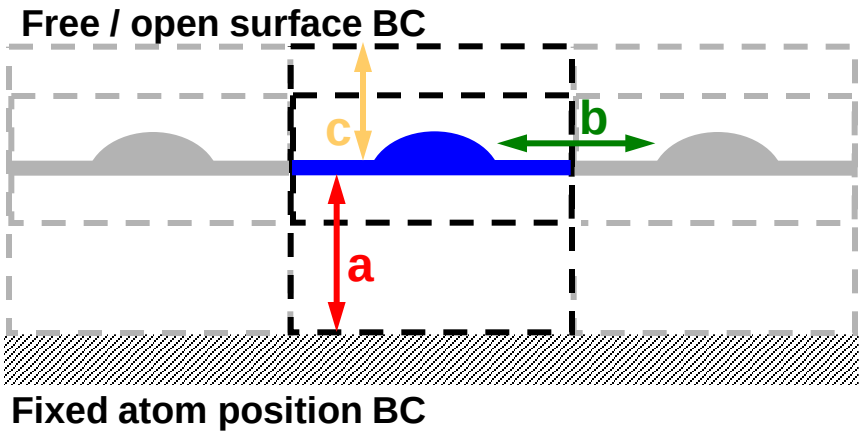
- Domain ratio *d/h* is fixed to 2
- Electronic domain always contains 2 mln atoms
- Strain domain contains up to 64 mln atoms
- Computations for deeply buried dot and dot array with free surface

Result: strain field is long-range!

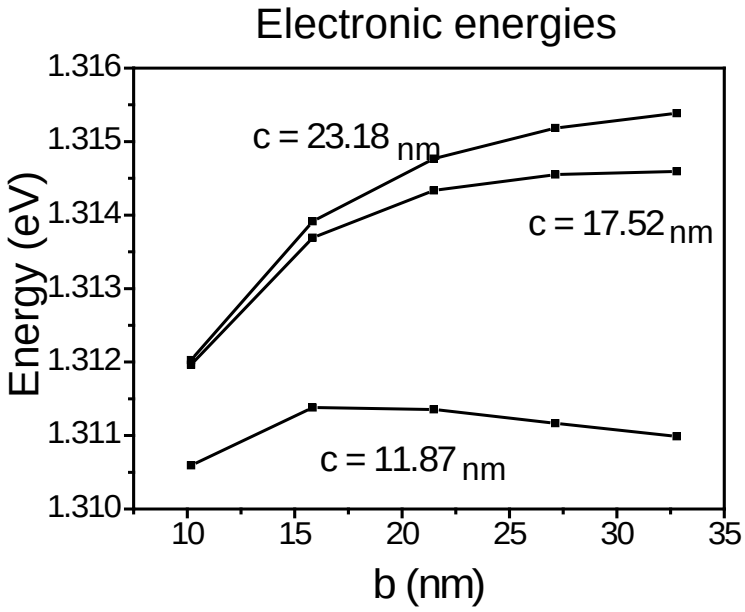
Arrays of quantum dots: neighbor distance and finite cap size

Cap thickness c parameter

Interdot distance b Measured from QD edge to edge



Base thickness a is large (To ensure convergence)



- Computed: the low-energy edge of the lowest electronic miniband
- Dots are coupled both via strain and quantum-mechanically
- Anomalous dependence for the thinnest cap is due to strong strain relaxation via the top surface of the sample

Summary

- Strain is the source of the creation of the InAs QDs on GaAs
- Strain is a long range phenomenon
- Strain reaches further vertically than horizontally
  - »Quantum dots will grow on top of each other
- Electron wavefunctions are confined to the central quantum dots and can be computed in a smaller domain