Nano 101
Quantum ~~Dots~~ WHAT?

Gerhard Klimeck
Technical Director
Network for Computational Nanotechnology (NCN)

Presentation Outline

- Classical Systems
  - Particles
  - Propagating Waves
  - Standing Waves
  - Chromatography
- Strange Experimental Results => The Advent of Quantum Mechanics
  - Discrete Optical Spectra
  - Photoelectric Effect
  - Particle-Wave Duality
- Quantum Dots
  - What is a Quantum Dot
  - Experimental Examples
  - Applications
- NEMO 3-D - Nanoelectronic Modeling
  - Multimillion Atom Simulations
  - Artificial Atoms and Artificial Molecules

Classical Macroscopic Particles

Properties:

- Have a finite extent
- Have a finite weight
- Are countable with integers

- continuous (ignoring atomic granularity)
- continuous (ignoring atomic granularity)
- discrete

Laws of Motion

- Classical Newtonian Mechanics

Interactions with other particles

- Energy continuity
- Momentum continuity

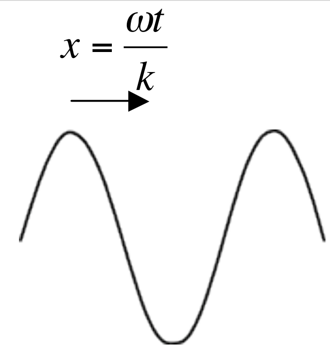
Example

- Billiard balls

Propagating Plane Waves

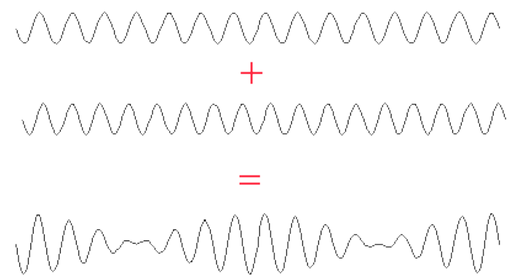
Properties:

- Have infinite extent
- Have finite wavelength
- Have a finite frequency



Laws of Motion $\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 x}{\partial x^2} = 0$

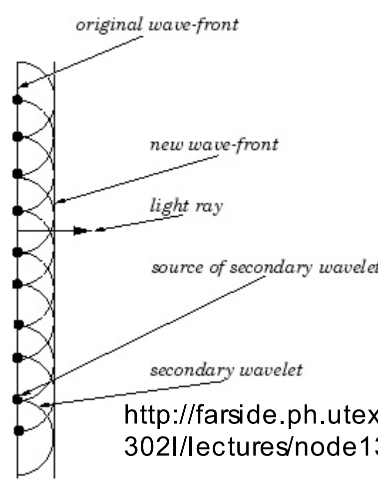
- Wave equation
- One solution $u = u_0 \sin(kx - \omega t) \quad c = \pm \omega/k = \pm \lambda f$



http://www.qmw.ac.uk/~zgap118/5/

Interactions with other waves / environment

- Coherent superposition
  => interference, constructive and destructive
  => one wave can cancel out another
- Huygens principle:
  one plane wave made up by many circular waves
  => diffraction
  => waves go around corners



http://farside.ph.utexas.edu/teaching/302l/lectures/node135.html

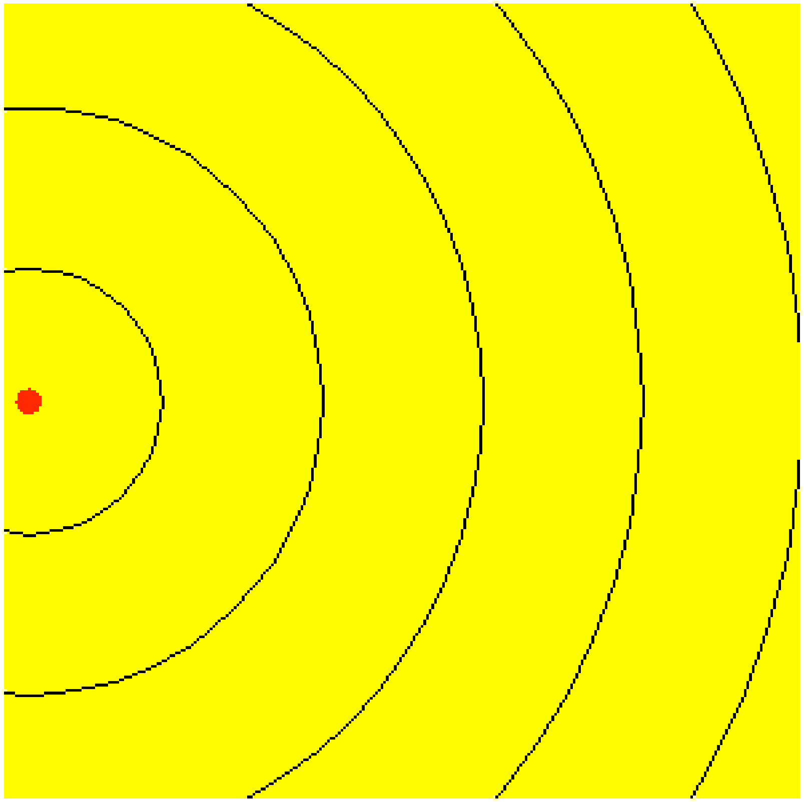
nanoHUB.org

online simulations and more

Huygens' Principle

- All waves can be represented by point sources

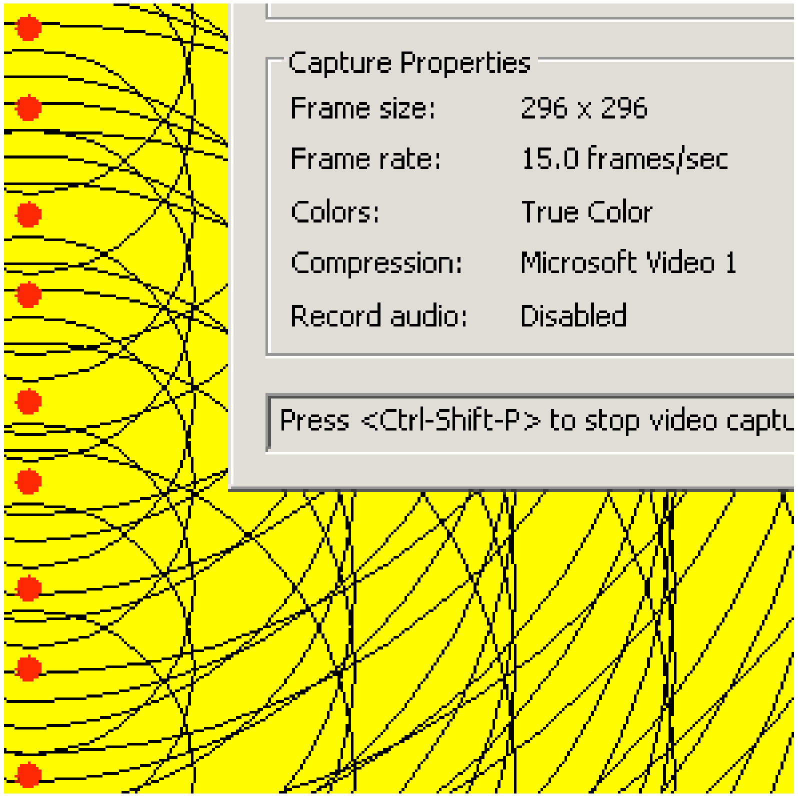
- This animation shows an example of a single point source



http://id.mind.net/~zona/mstm/physics/waves/propagatio

Huygens' Principle

- All waves can be represented by point sources
- This animation shows an example of multiple single point sources creating a wavefront.



http://id.mind.net/~zona/mstm/physics/waves/propagatio

Propagating Plane Waves
Light is an Electromagnetic Wave

Properties:

- Have infinite extent — • Not countable
- Have finite wavelength — • Continuous
- Have a finite frequency — • Continuous

Laws of Motion

- Wave equation $$\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 x}{\partial x^2} = 0$$
- One solution $$u = u_0 \sin(kx - \omega t) \qquad c = \pm \omega/k = \pm \lambda f$$

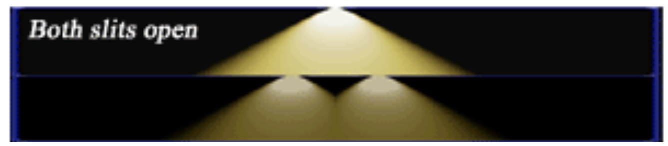
Interactions with other waves / environment

- Coherent superposition
  => interference, constructive and destructive
  => one wave can cancel out another
- Huygens principle:
  one plane wave made up by many circular waves
  => diffraction
  => light goes around corners

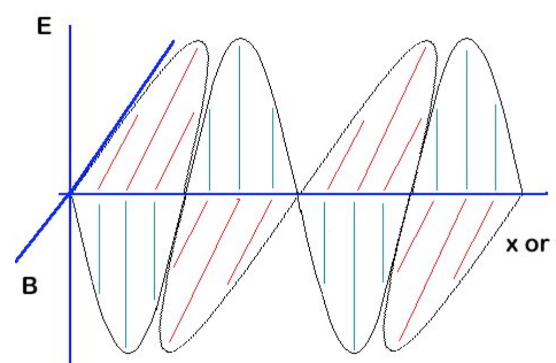
Accepted Proof:

- Light is an electromagnetic wave

Double Slit Experiment



http://en.wikipedia.org/wiki/Double-slit_experiment



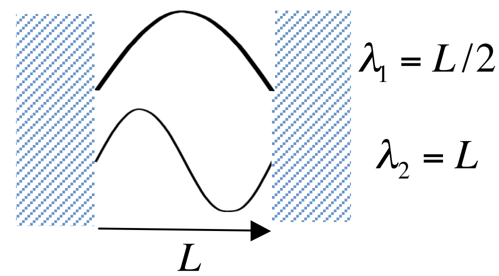
http://www.qmw.ac.uk/~zgap118/2/

Standing Waves

Properties:

- Have finite extent
- Have discrete wavelengths
- Have discrete frequencies

- Countable in 1/2 wavelength
- Integer multiples
- Integer fractions



Laws of Motion

- Wave equation
- One solution

$$\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 x}{\partial x^2} = 0$$

$$u = \begin{cases} u_0 \sin(kx - \omega t);\ 0 \le x \le L \\ 0; \quad x < 0; x > L \end{cases}$$

$$k_j = j\frac{\pi}{L}$$

- Quantized momentum k_j

Interactions with other waves / environment

- Coherent superposition
  => e.g. sounds add in an instrument
- A standing wave is a resonator
- one resonator can couple to another
  => e.g. string <=> guitar
  => energy is transferred between resonators
  => energy conservation
- resonators must be “in-tune”
  => momentum conservation

Frequency Content of Light

- “White” light consists of a broad spectrum of colors
- Each individual color is associated with a particular frequency of wave
- A prism can dissect white light into its frequency components

- Is there some information in this kind of frequency spectrum?
  => chromatography

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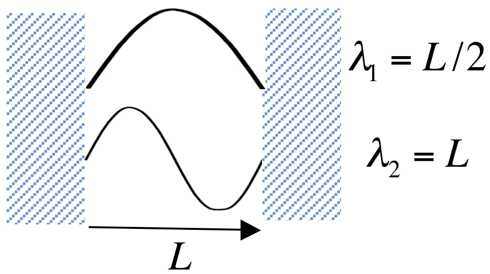

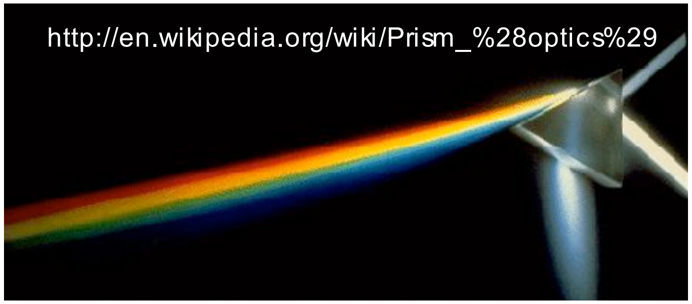

- Strange Experimental Results => The Advent of Quantum Mechanics
  - Discrete Optical Spectra
  - Photoelectric Effect
  - Particle-Wave Duality
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  - What is a Quantum Dot
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Strange Experimental Observations
The Advent of Quantum Mechanics

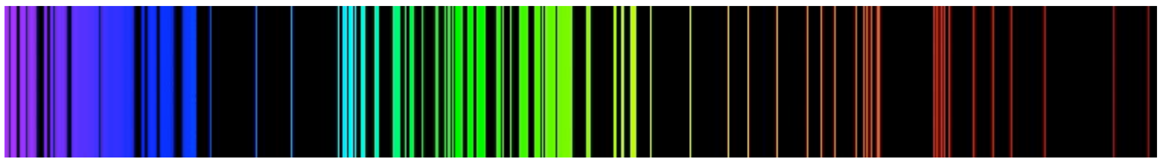
Discrete light spectrum:

- Light emitted from hot elemental materials has a discrete spectrum
- The spectrum is characteristic for the material (fingerprint)

Images from: http://en.wikipedia.org

- E.g.: H spectrum

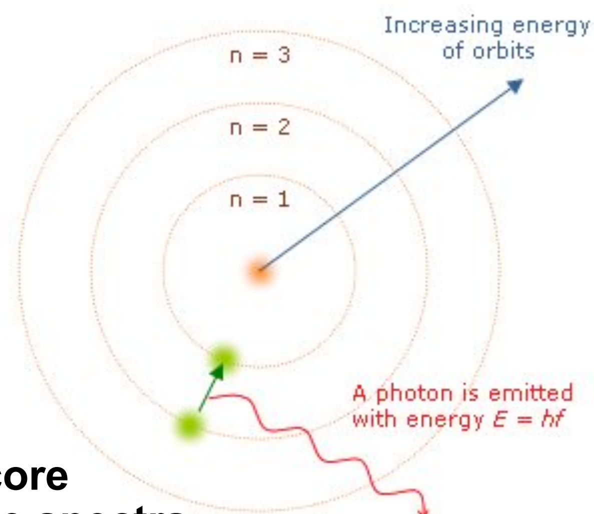
- E.g.: Iron spectrum

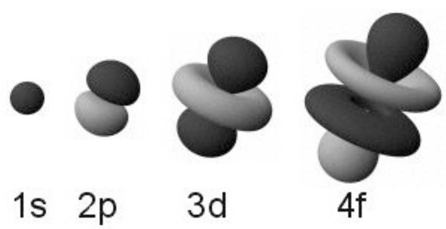


- E.g. application - bright yellow Na lamps
  => lot of excitation energy converted into single frequency

Development of atomic models

- Bohr atom model - electrons in looping orbits
- Quantum mechanical model



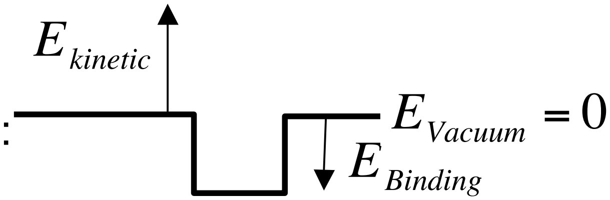


=> electrons are standing waves bound to a core
=> discrete transition energies lead to discrete spectra

Strange Experimental Observations
The Advent of Quantum Mechanics

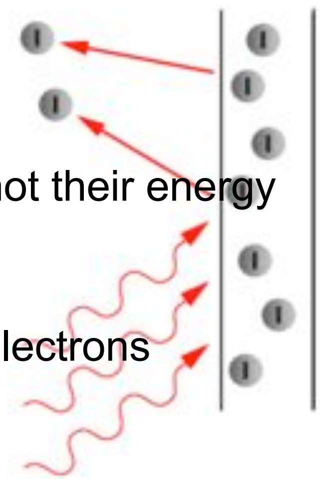
Photoelectric Effect:

- Light can eject electrons from a clean metal
- Observed by many researchers but not explained for 55 years: 1839, 1873, 1887, 1899, 1901
  see details: http://en.wikipedia.org/wiki/Photoelectric_effect



Unexplained problems:

- Electrons emitted immediately, no time lag
- Increasing light intensity increases number of electrons but not their energy
- Red light will not cause emission, no matter what intensity
- Weak violet light will eject few electrons with high energy
  => Light had to have a minimum frequency / color to excite electrons
  f_m
- => Emitted electrons have light dependent energy
  $\Delta E \propto (f - f_m)$



http://en.wikipedia.org/wiki/Photoelectric_effect

The solution in 1905 (Nobel prize for Einstein in 1921)

$$E = hf$$

- Light can be described by discrete particles of discrete energy
- Planck's constant - h
- Light energy is not divisible
- Have to have minimum energy to kick out an electron from the bound state

Light consists of particles

Photons

$$E_{Binding} = hf_m \qquad E_{kinetic} = E_{light} - E_{Binding} = h\left(f_{light} - f_m\right) \geq 0$$

Wave - Particle Duality

All particles have a wave property

- Can interfere
- Can diffract
- Can form standing waves

All waves have particle properties

- Have momentum
- Have an energy
- Can be created and destroyed

Typical descriptions:

- Energy E, frequency f, Momentum k
- A set of discrete quantum numbers

- Choose wave/particle description according to problem

More Mind Games

- Electrons in atoms are attracted / confined by the atomic core
  => electrons are
  - Quantized in energy
  - Located in orbitals

- What if we could:
  - Confine electrons to a small, man-made space?
  - Make sure the material is “clean”

- Sounds like an “artificial atom”

=> **Quantum Dot**

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Pain Pointer

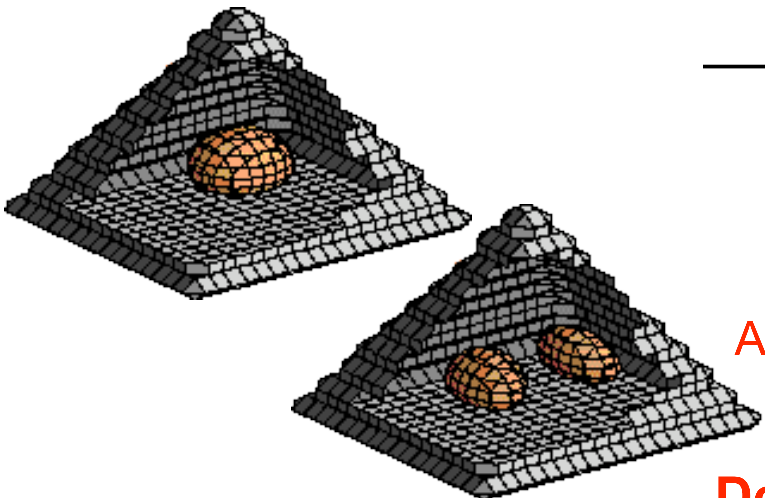
What is a Quantum Dot ?
Basic Application Mechanisms

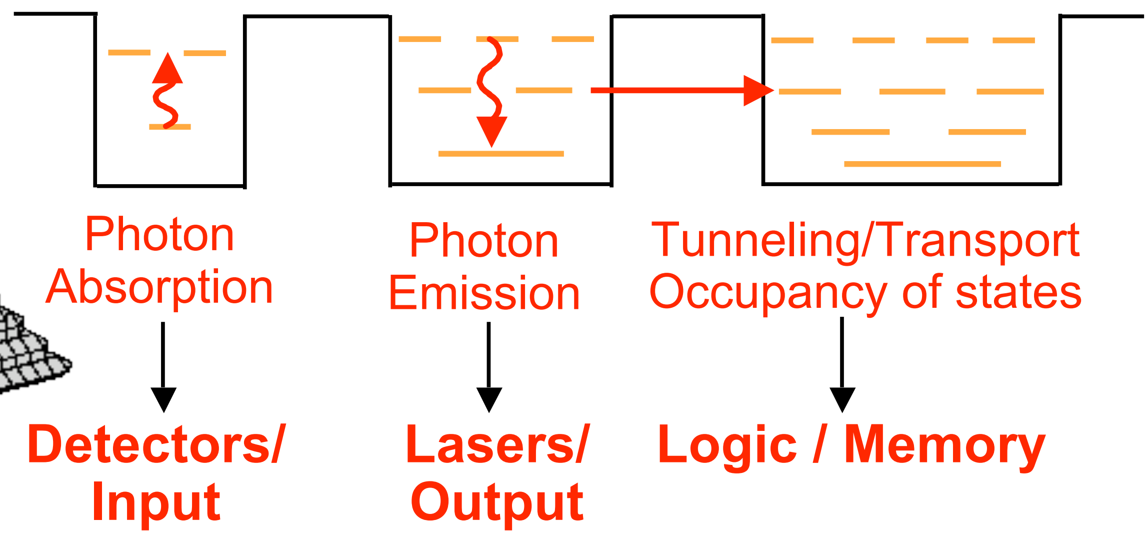
Physical Structure:

- **Well conducting / low energy domain surrounded in all 3 dim. by low conducting / high energy region(s)**
- **Domain size on the nanometer scale**

Electronic structure:

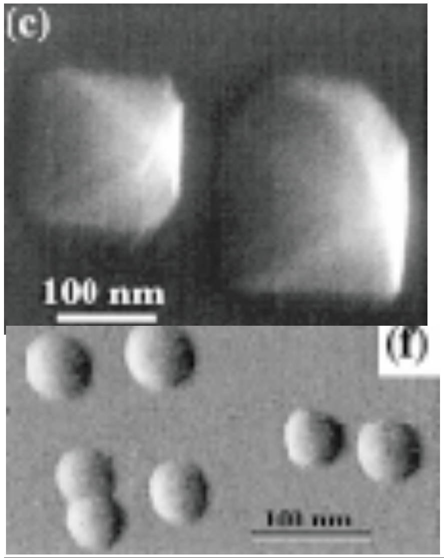
- **Electron energy may be quantized -> artificial atoms (coupled QD->molecule)**
- **Contains a countable number of electrons**





Quantum dots are artificial atoms that can be custom designed for a variety of applications

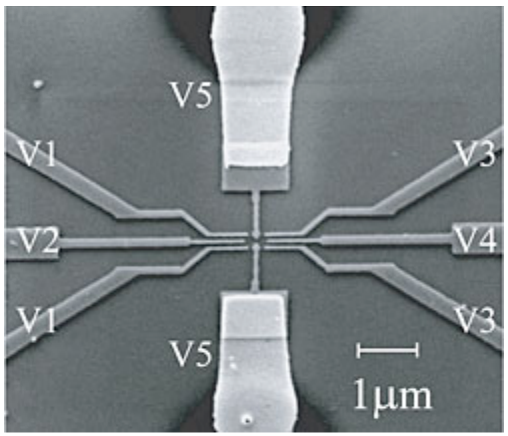
QD Example Implementations



Self-assembled , InGaAs on GaAs.

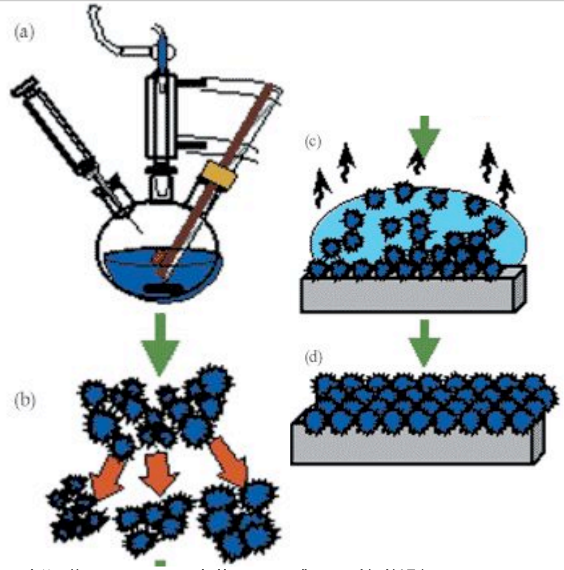
Pyramidal or dome shaped

R.Leon,JPL(1998)



Electrostatic Gates, GaAs, Si, Ge
Create electron puddles

Source: http://www.spectrum.ieee.org/WEBONLY/wonews/aug04/0804ndot.html



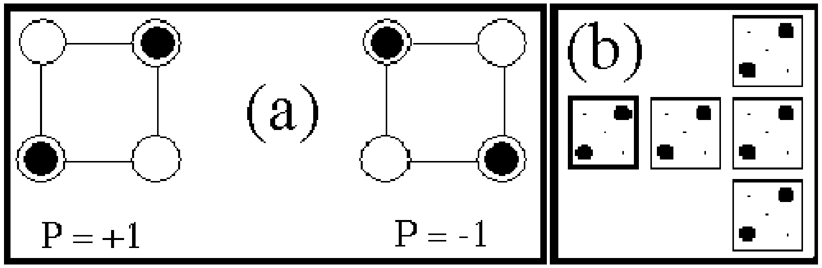
Colloidal, CdSe, ZnSe

http://www.research.ibm.com/journal/rd/451

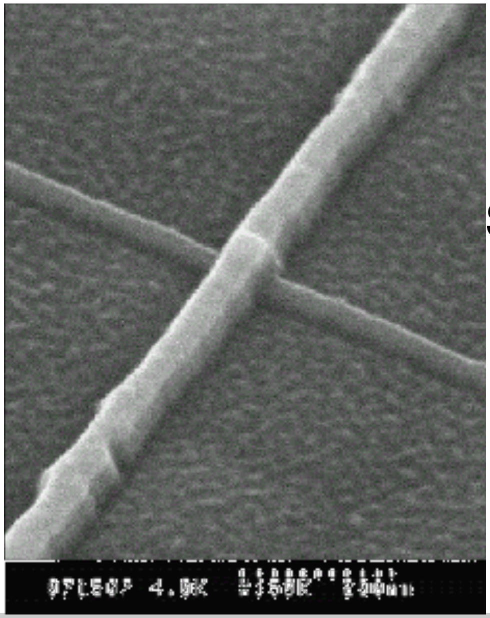
Fluorescence induced by exposure to ultraviolet light in vials containing various sized cadmium selenide (CdSe) quantum dots.
Source: http://en.wikipedia.org/wiki/Fluorescent ß

Quantum Dot Applications

- **Memory:**
  Store discrete charge in potential wells.
- **Transistors:**
  Use discreteness of channel conduction.
- **Logic:**
  Use electrostatically coupled quantum dots.

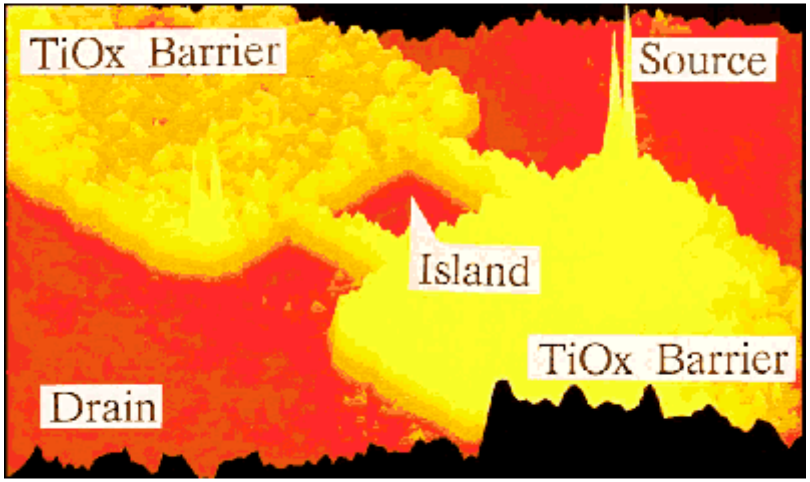


Lent, Porod @ Notre Dame: Quantum Cellular automata, electrostatically coupled quantum dots.



Chou @ Princeton Room Temp. Single Electron Memory

Hitachi: 128Mbit Integration demonstrated

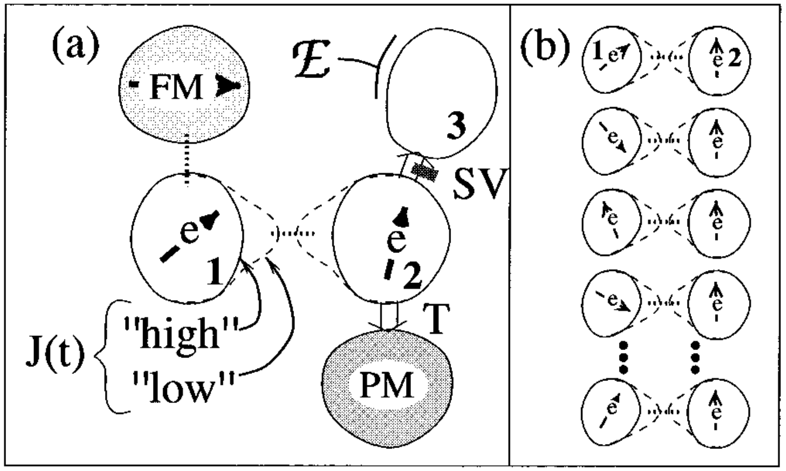


Harris @ Stanford: Room temperature single electron transistor

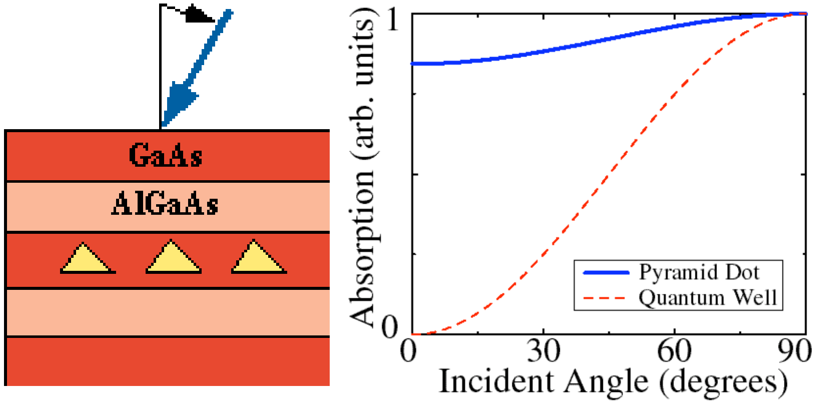
Quantum Dot Applications 2

- **Medical Markers:**
  Inject body with optical markers that are attached / adsorbed to particular tissue
- **Quantum Computing:**
  Process coherent states of charge, spin, or optical interactions
- **Infrared Detectors:**
  Can absorb light at all angles

Colloidal Dots can be used as implantet optical markers



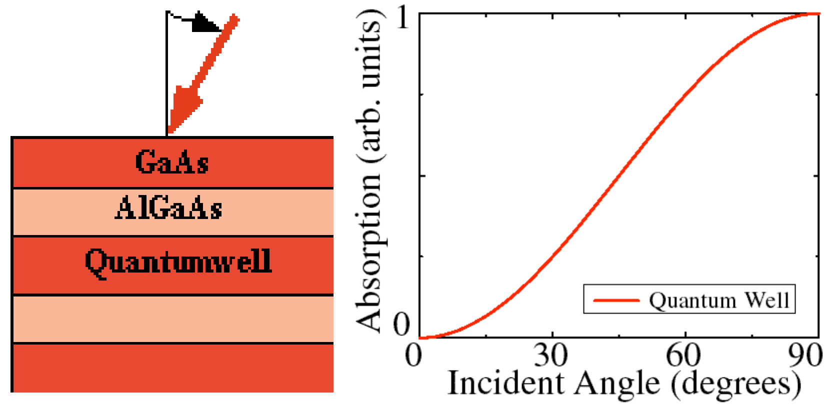
QDs for Quantum Computing



Quantum Dots: Absorption has weak incidence angle dependence

Quantum Dots as Optical Detectors

- **Problem:**
  Quantum wells are “blind” to light impinging orthogonal to the detector surface.
- **Standard Solution:**
  Need gratings to turn the light
- **New Approach:**
  Quantum dots have a built-in anisotropy and state quantization in all three dimensions
  -> absorption at all angles

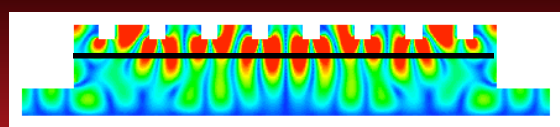


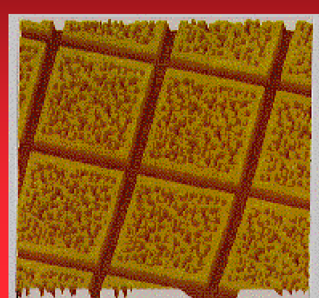
Quantum Wells: Absorption has strong incidence angle dependence

Standard Solution:

Grating

Electromagnetic Modeling

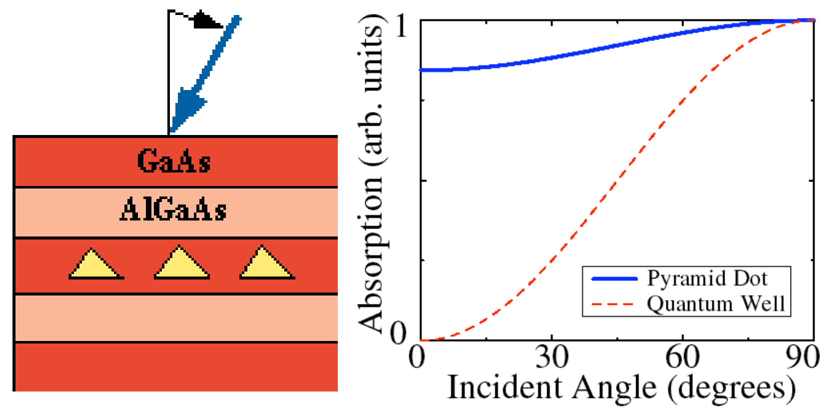




electric field models

↓

optimized light coupling



Quantum Dots: Absorption has weak incidence angle dependence

Lighting

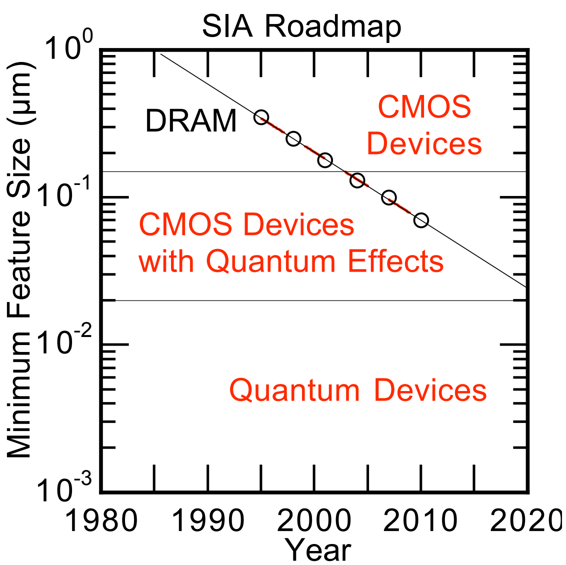
- Quantum-dot LEDs
  - Seem to be key to advances in the fields of full-color, flat-panel displays and backlighting
- QD emits a color based on its size
  - Smaller dots emit shorter wavelengths, such as blue, which, in the past, has been difficult to attain
  - Larger dots emit longer wavelengths, like red

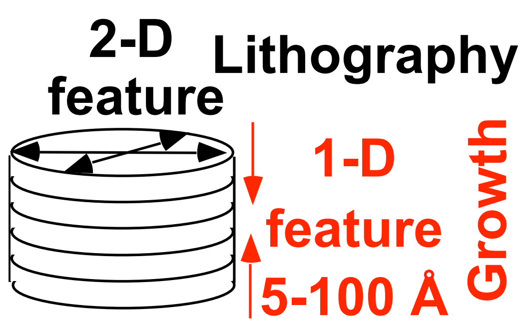
Fluorescence induced by exposure to ultraviolet light in vials containing various sized cadmium selenide (CdSe) quantum dots.

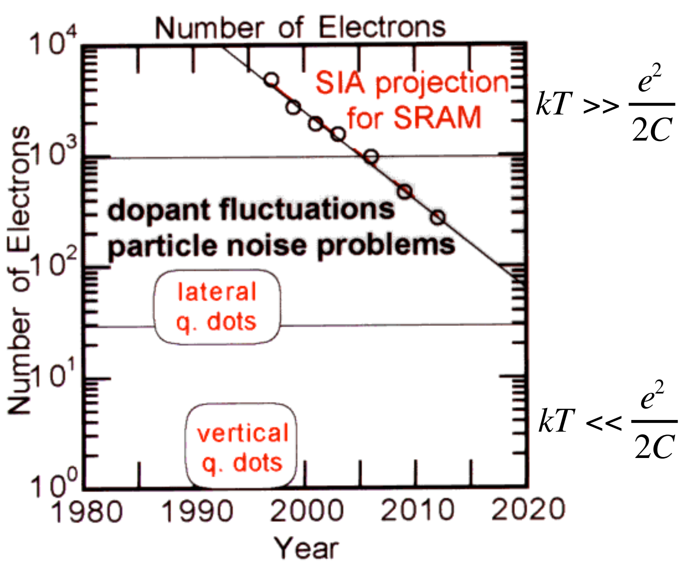
Source: http://en.wikipedia.org/wiki/Fluorescent

Moore's Law (loosely formulated):

- **Overall device performance doubles every 18 months**
- **Historically true for over 20 years**
- **Technically achieved by**
  - **Making device features ever smaller**
    => devices become faster
  - **Making wafer ever larger**
    => reducing or maintainig the overall cost per chip







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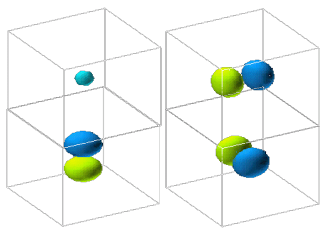
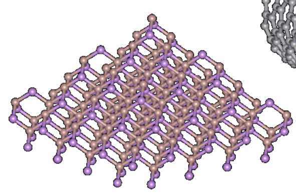
Pain Pointer

NEMO 3-D Technical Approach



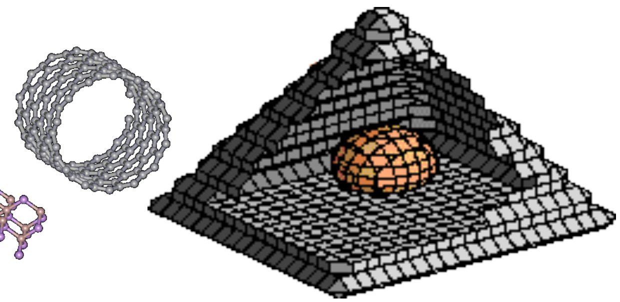
Atomic Orbitals
size: 0.2nm

+



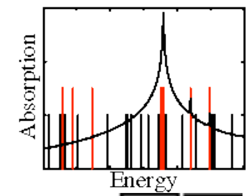
Structure
Millions of atoms

→

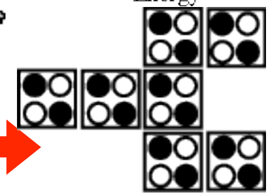


Nanoscale Quantum States
(Artificial Atoms, size 20nm)

→



Designed
Optical
Transitions
Sensors



Quantum Dot
Arrays
Computing

Problem:

Nanoscale device simulation requirements:

- Cannot use bulk / jellium descriptions, need description of the material atom by atom
  => use pseudo-potential or local orbitals
- Consider finite extend, not infinitely periodic
  => local orbital approach
- Need to include about one million atoms.
  => need massively parallel computers
- The design space is huge: choice of materials, compositions, doping, size, shape.
  => need a design tool

Approach:

- Use local orbital description for individual atoms in arbitrary crystal / bonding configuration
  - Use s, p, and d orbitals.
  - Use genetic algorithm to determine material parameter fitting
- Compute mechanical strain in the system.
- Develop efficient parallel algorithms to generate eigenvalues/vectors of very large matrices (N=40million for a 2 million atom system).
- Develop prototype for a graphical user interface based nanoelectronic modeling tool (NEMO-3D)

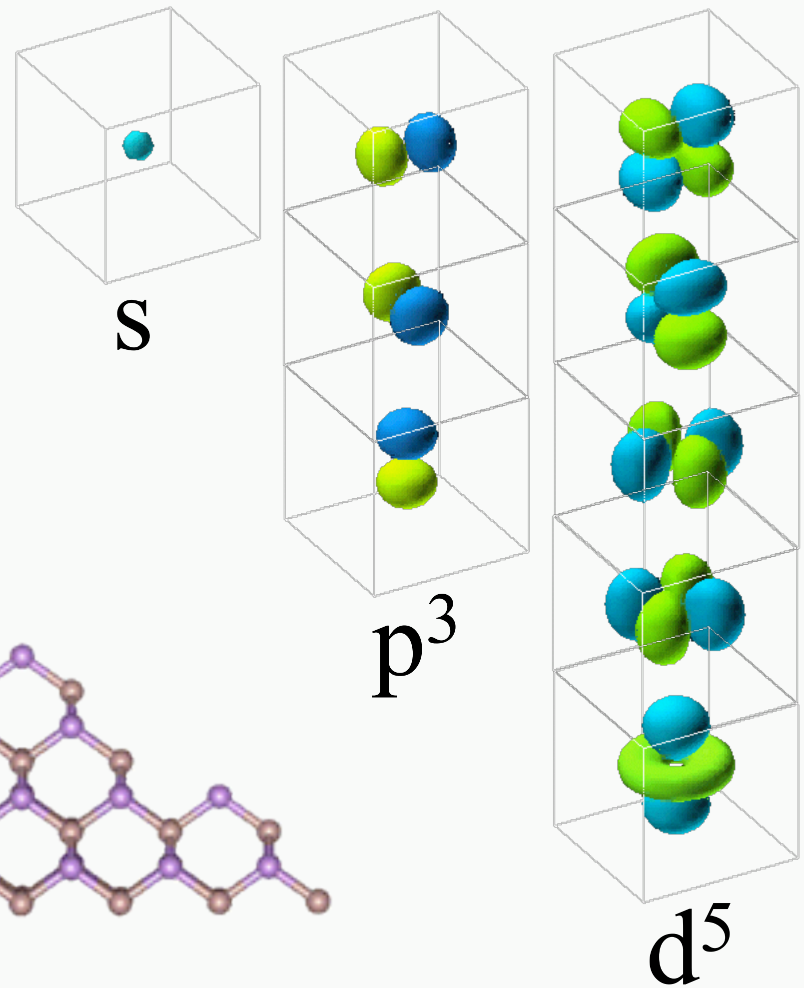
Realistic material description at the atomic level enables simulation of realistic nanoelectronic devices.

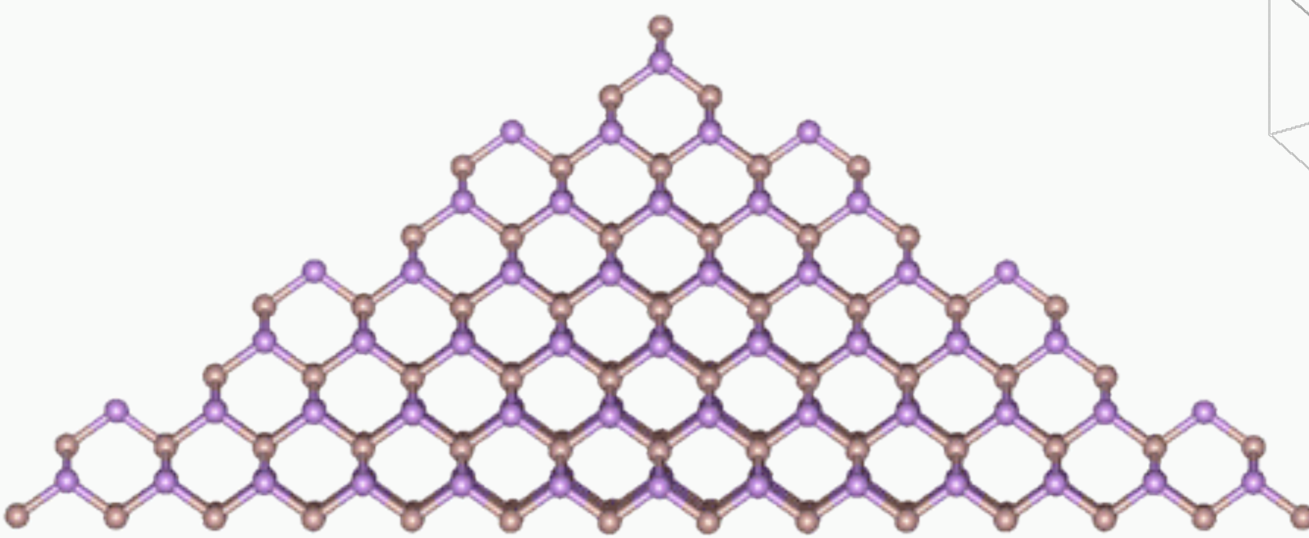
Atomistic Tight-Binding Hamiltonian

$$\psi_{i,j,k} = \sum_{l}^{orbitals} C_{i,j,k}^{l} \phi_l$$

$$\phi_l = s, p^3, d^5$$

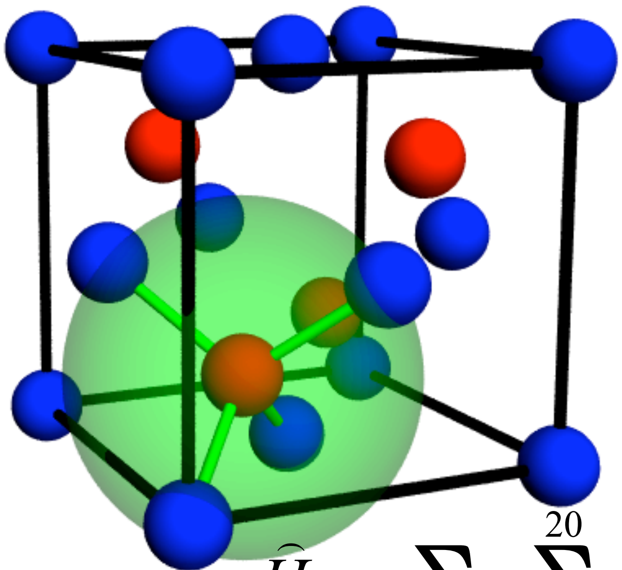
Wavefunction Basis





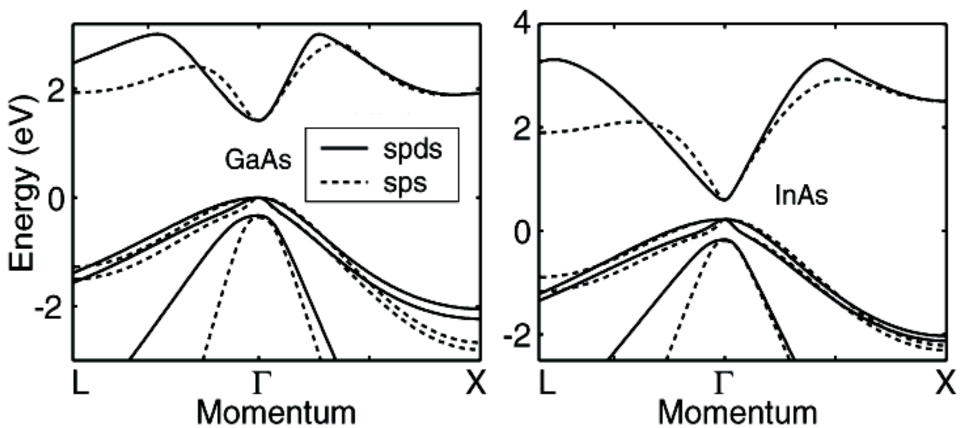
Crystalline Structure

Nearest-Neighbor sp3d5s* Model



- Realistic zinc-blende lattice
- Each atom has 10 spin-degenerate orbitals ($sp^3d^5s^*$)
- Each atom has 4 nearest neighbors
- TB parameters found by fitting of bulk band structure to experiment

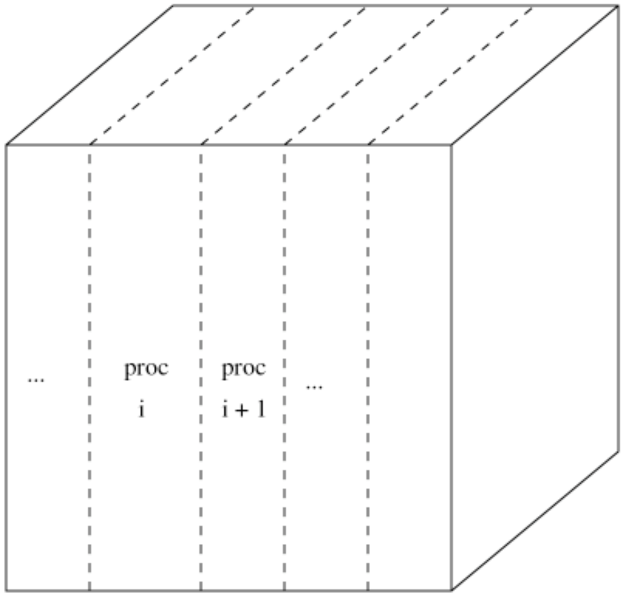
$$\hat{H} = \sum_{atoms\ R} \sum_{\substack{\alpha=1 \\ bands}}^{20} \varepsilon_{R\alpha} c^{+}_{R\alpha} c_{R\alpha} + \sum_{atoms\ R} \sum_{atoms\ R'=1}^{4nn} \sum_{\substack{\alpha=1 \\ bands}}^{20} \sum_{\substack{\alpha'=1 \\ bands}}^{20} t_{R\alpha,R'\alpha'} c^{+}_{R\alpha} c_{R'\alpha'}$$

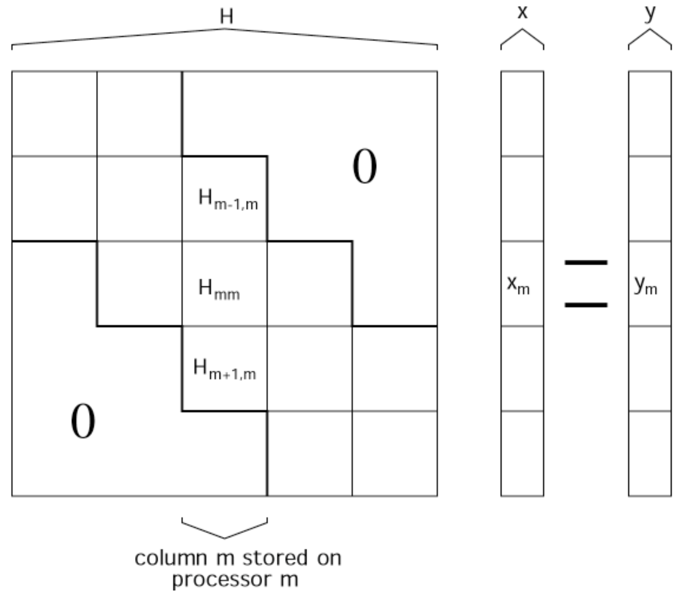


Systems with up to 21 million atoms

Matrix order: 4×10^8
Lanczos Diagonalization

Parallelization and Methods





- Divide Simulation domain into slices.
- Communication only from one slice to the next (nearest neighbor)
- Communication overhead across the surfaces of the slices.

- Limiting operation:
  complex sparse matrix-vector multiplication
- Enable Hamiltonian storage or re-computation on the fly.

- Electronic structure needs eigenvalues and eigenvectors. Matrix is Hermitian
- NEMO 3-D methods:
  - Standard 2-pass Lanczos
  - PARPACK about 10x slower
  - Folded Spectrum Method (Zunger), also typically slower than Lanczos

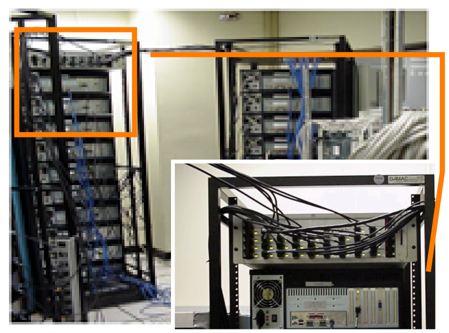
From Beowulf Concept (JPL, Tom Sterling) to Commodity Products in 4 Generations

Hyglac (1997)
16 Pentium Pros 200MHz
128 MB RAM per node
2 GB total
5GB Disc per node
80 GB total
100 Mb/s ethernet crossbar
Linux, MPI
3.2GFlops

Gordon Bell Prize 1997

Nimrod (1999)
32 Pentium IIIs 450MHz
512 MB RAM per node
16 GB total
8GB Disc per node
256 GB total
100 Mb/s ethernet crossbar
Linux, MPI
14.4 GFlops

Pluto (2001)
64 Pentium IIIs 800MHz
dual CPUs
2 GB RAM per node
64 GB total
10 GB Disc per node
320 GB total
2 Gb/s Myricom crossbar
Linux, MPI
51.2 GFlops

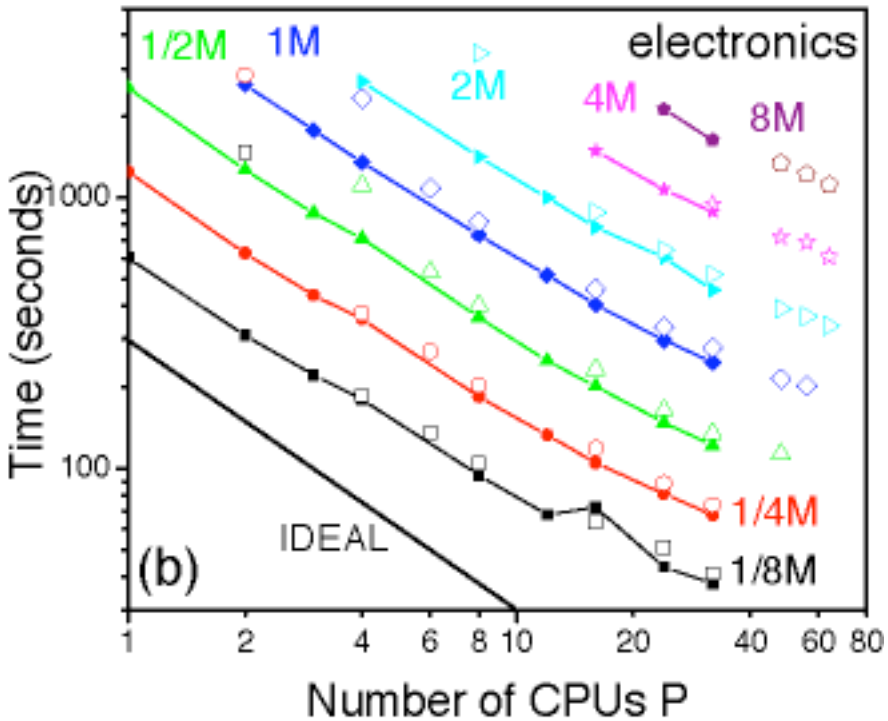


NewYork (2002)
66 Xserve G4 1GHz
1GB RAM per node
33 GB total
60 GB Disc per node
2 TB total
100 Mb/s ethernet crossbar
MAC OS X, MPI
495GFlops

Affordable Supercomputer
for ~$100k

Parallelization Benchmark Apple G5

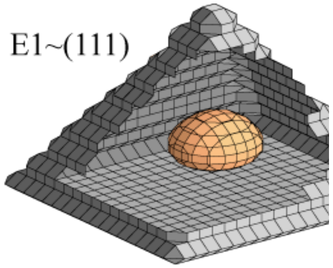
G5 Apple cluster: a 32 node G5 Xserver Apple cluster at JPL, with nodes consisting of dual 2GHz PowerPC G5, 2GB RAM, Dual Gigabit Ethernet.



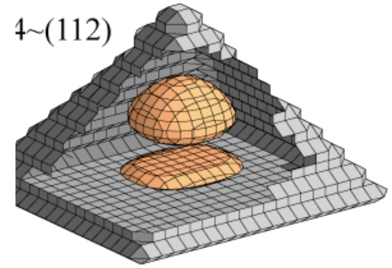
Electronics scale well

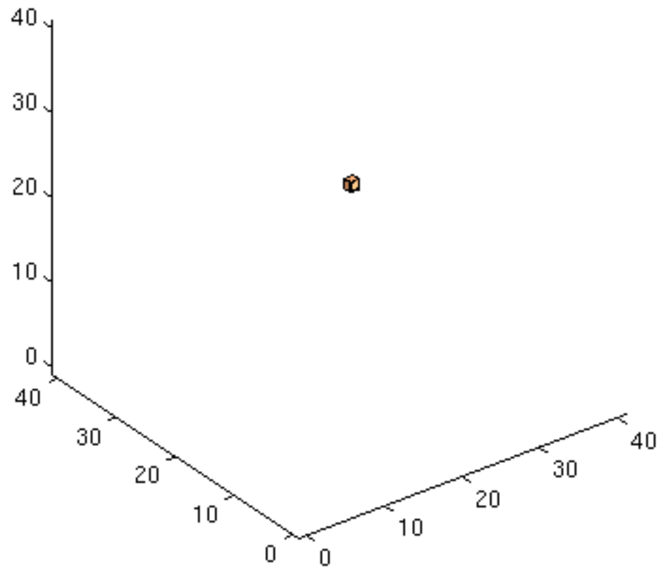
Some Wavefunctions of a Pyramidal Quantum Dto

E1~(111)

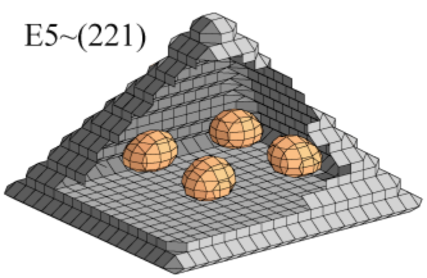


4~(112)

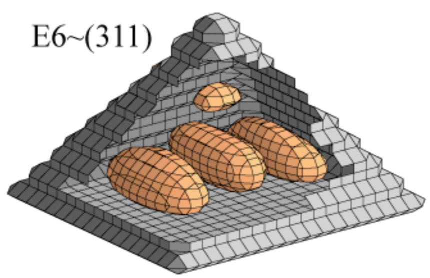




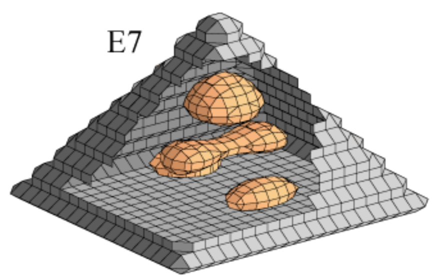
E5~(221)



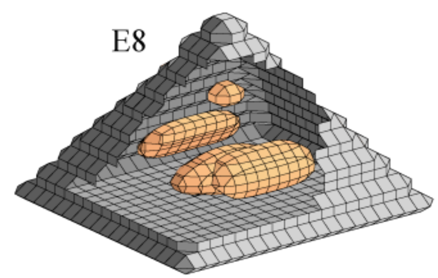
E6~(311)



E7



E8



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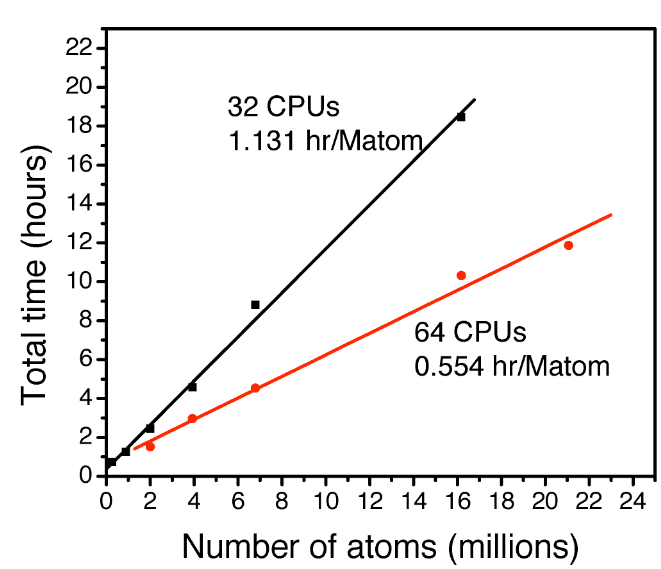
HPC and Visualization

NEMO 3-D: Electronic structure for tens of Million Atoms

NCN Objective:
- Engage computational scientists
- Deploy new community codes
- Advance the state-of-the-art in nano simulation through HPC

Approach:
- Identify a numerically challenging nano simulation problem
- Multidisciplinary team: ECE, CS, ITaP: 2 fac, 2 s/w prof, 1 post-doc,5 students

Performed on NSF Teragrid



Nano-Problem:
- Atomistic quantum dot simulations

Computational Problem
- Conjugate grad. real $O(3x10^8)$ 100Ma
- Interior eigenvect comlx $O(4x10^8)$ 20Ma
- Efficient parallelization

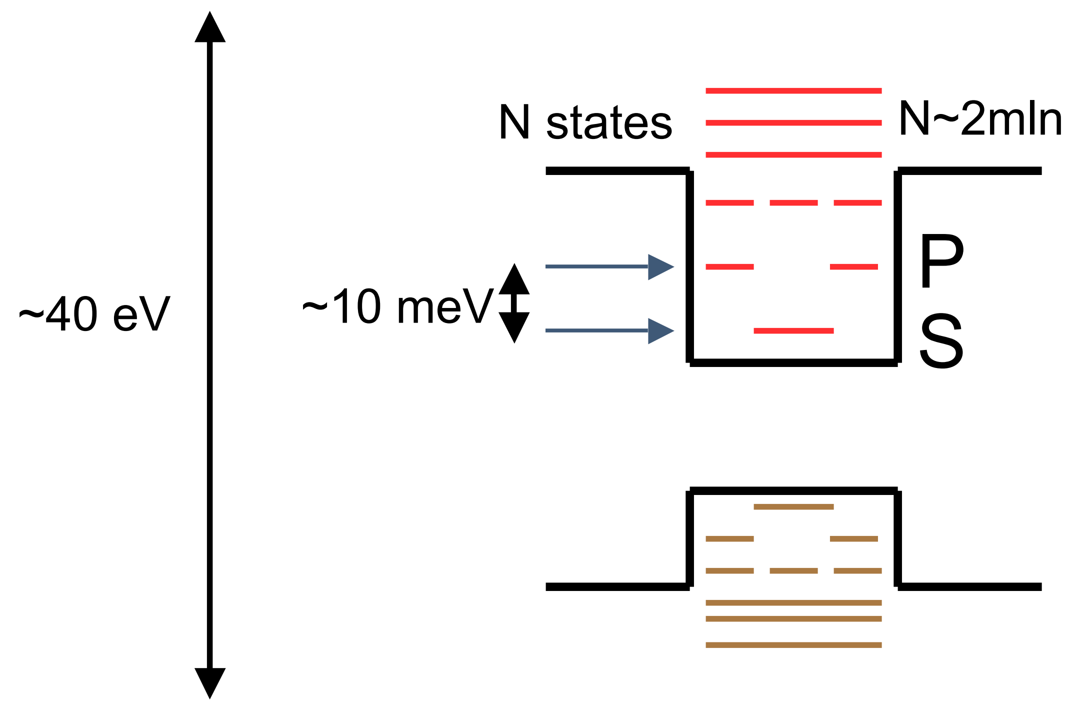
Status one year ago:
- Strain 16Ma - $O(4.8x10^7)$
- Eigenvalues: 9Ma - $O(1.8x10^7)$
- Eigenvectors: 0.1Ma - $O(2x10^6)$

Result / Demonstrations / Impact:
- Algorithm, performance and memory utilization improvements
- Developed 3D volume rendering tool
- 64 Ma strain, $O(1.8x10^8)$,vol $(110nm)^3$
- 21 Ma electronics - value and vector $O(4.2x10^8)$, $(78nm)^3$ or $15x178x178nm^3$
- Studied long range strain
- Studied coupled quantum dots
- New details through visualizations

Computed Electronic in a realistic structure of $(78nm)^3$ volume

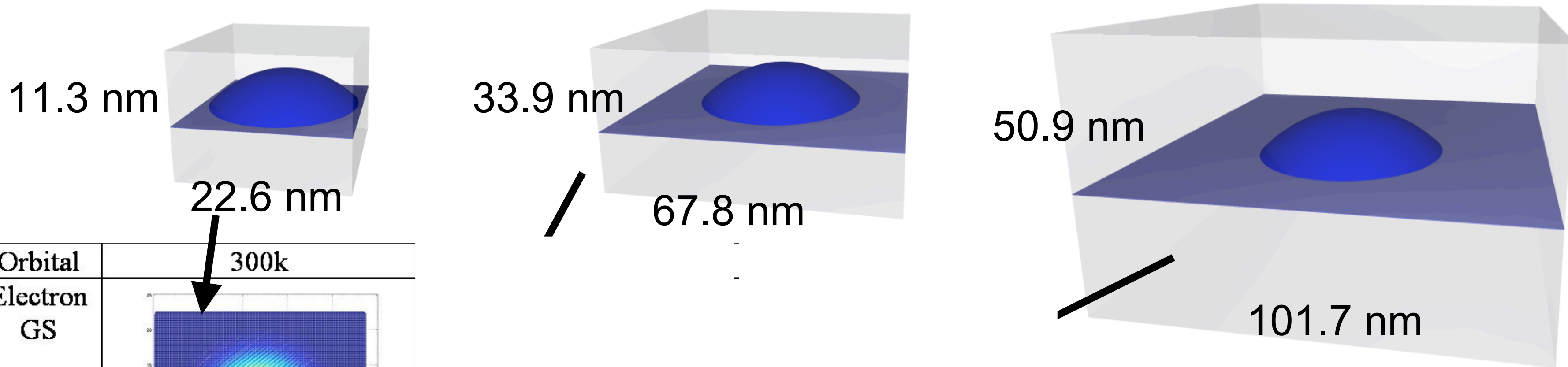
Proof of Concept

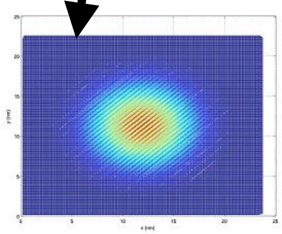
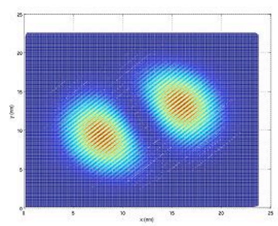
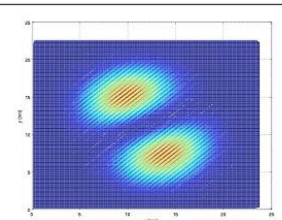
Extraction of Targeted Interior Eigenstates

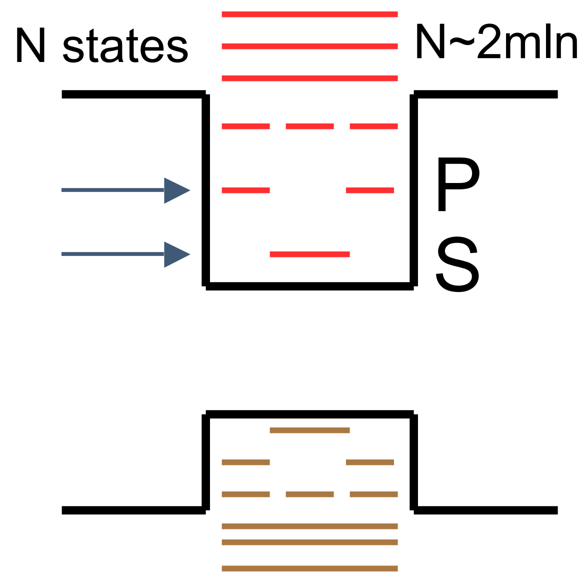


Proof of Concept

Extraction of Targeted Interior Eigenstates



Orbital	300k
Electron GS	
Electron 1ES	
Electron 2ES	



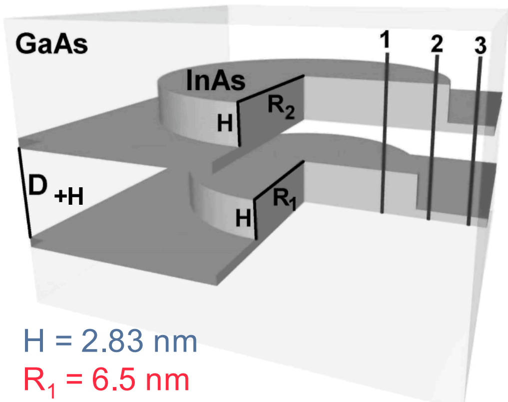
Unique and targeted eigenstates of correct symmetry
can be computed in all electronic computational domains

Presentation Outline

- Classical Systems
  - Particles
  - Propagating Waves
  - Standing Waves
  - Chromatography
- Strange Experimental Results => The Advent of Quantum Mechanics
  - Discrete Optical Spectra
  - Photoelectric Effect
  - Particle-Wave Duality
- Quantum Dots
  - What is a Quantum Dot
  - Experimental Examples
  - Applications
- NEMO 3-D - Nanoelectronic Modeling
  - Multimillion Atom Simulations
  - Artificial Atoms and Artificial Molecules

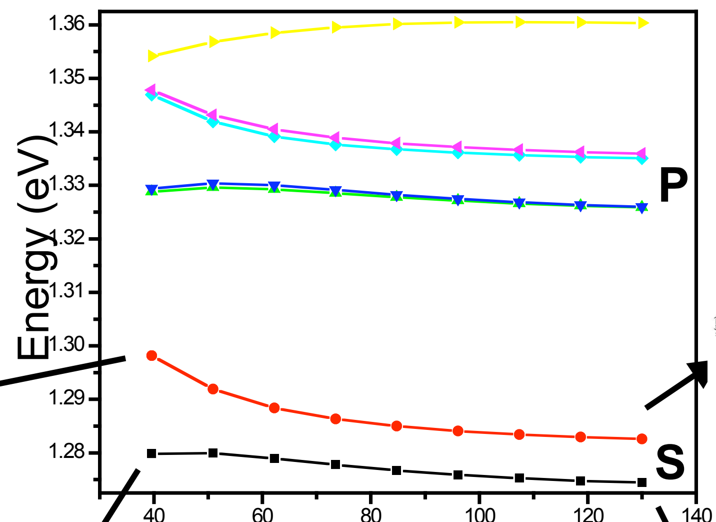
Pain Pointer

Vertically Coupled Two-Dot Molecule

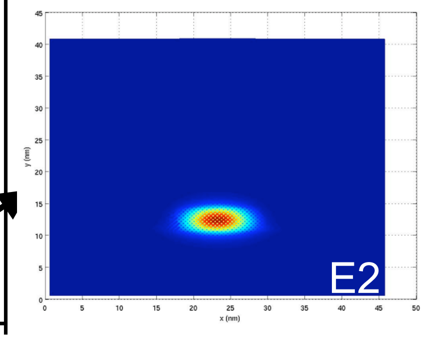


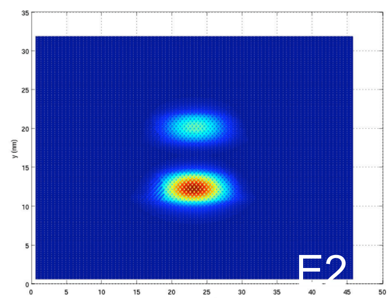
H = 2.83 nm
R_1 = 6.5 nm
R_2 = 6.96 nm
D IS A PARAMETER

ELECTRONIC QUANTUM-MOLECULAR ENERGIES



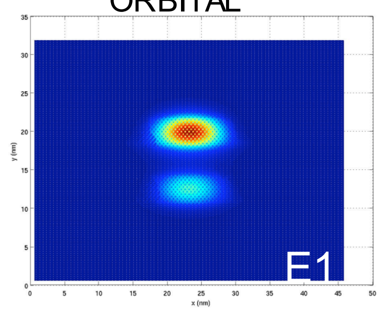
ORBITALS OF UNCOUPLED DOTS

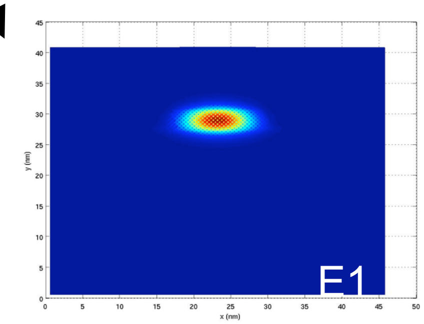




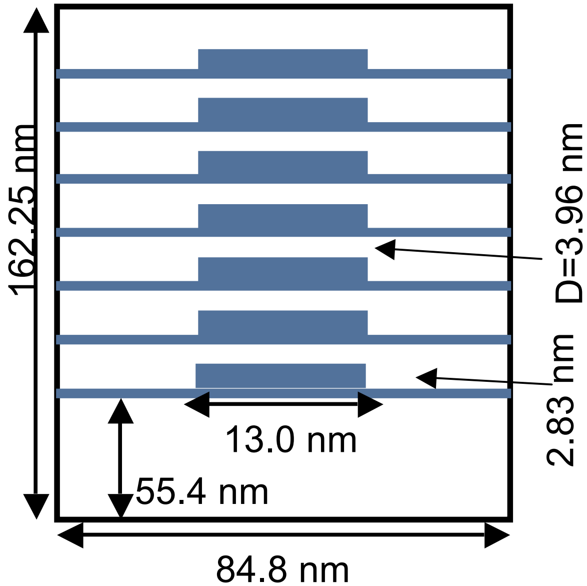
ANTIBONDING ORBITAL

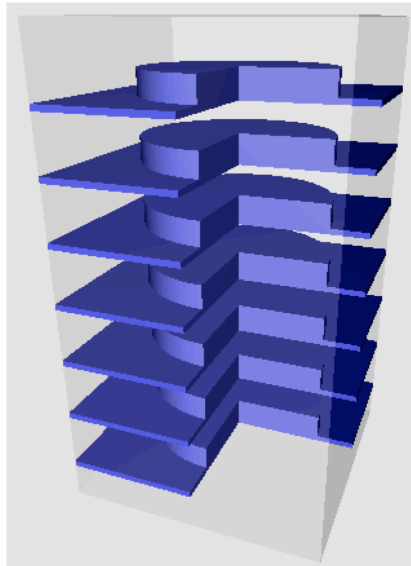
BONDING ORBITAL





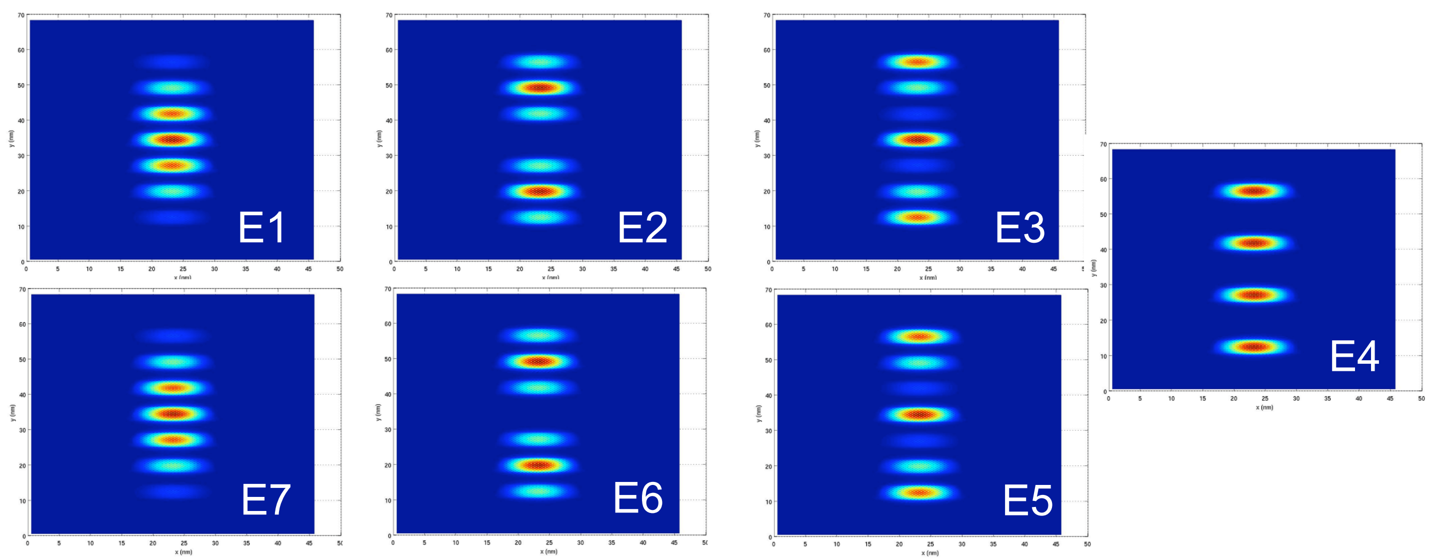
Vertically Coupled Seven-Dot Molecule
Identical dots





- Application in lasers
- Strain: 44.7 Ma
- Electronics: 6.1 Ma

- 7 Identical dots, without strain => symmetric miniband with 7 states
- Can derive this analytically from 1 dot simulations



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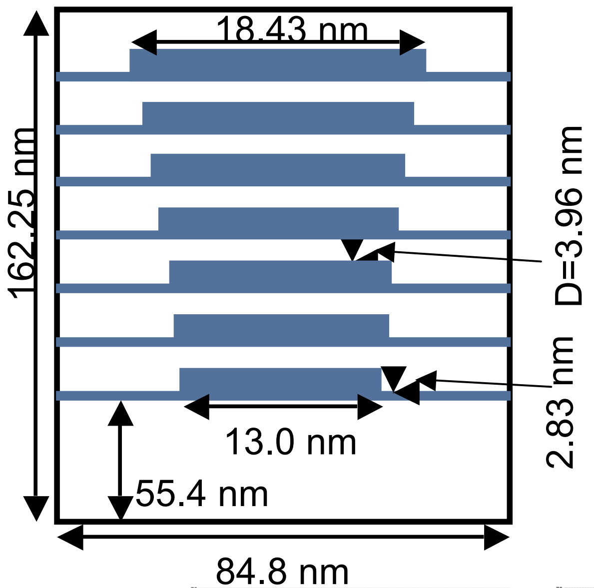
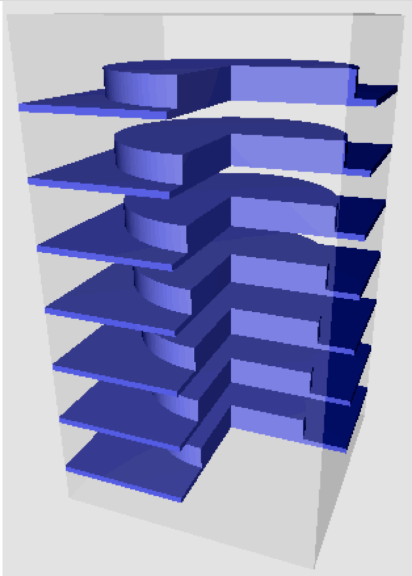
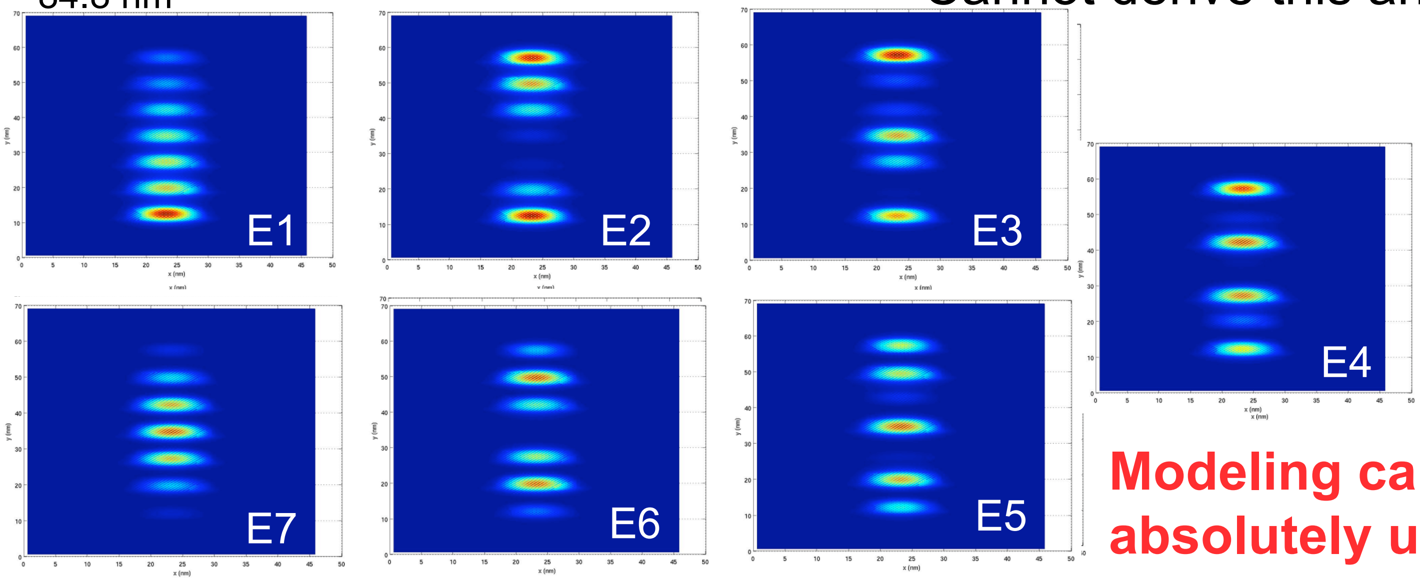
Vertically Coupled Seven-Dot Molecule
Growth asymmetry => Non-identical dots





- Application in lasers
- Strain: 44.7 Ma
- Electronics: 6.1 Ma

- Non-identical dots, higher dots have larger diameter
- Miniband broken
- Ground state in the BOTTOM!
- Cannot derive this analytically!



Modeling capability absolutely unique!!

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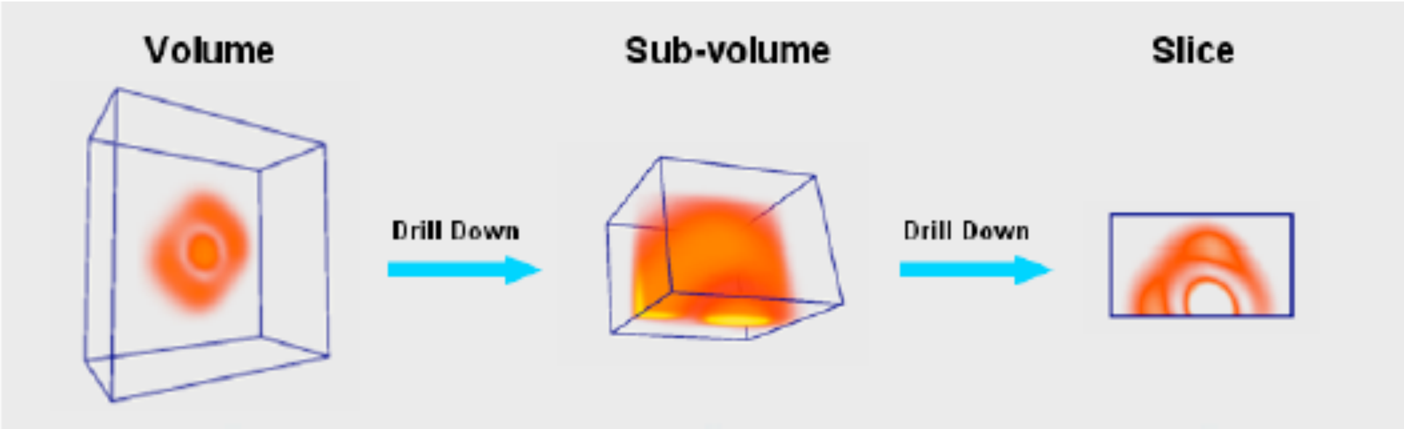
VolQD
Million Atom Volume Rendering on a single GPU

Objective/Problem - Requirements:
- Interactive volume data rendering
- Realistic crystals
- Crystal is not a space-filling mesh
- Need to drill down into data
- Would like to work on single CPU

Approach:
- Utilize Graphics Processing Unit-GPU
- Develop a visualization tool-box

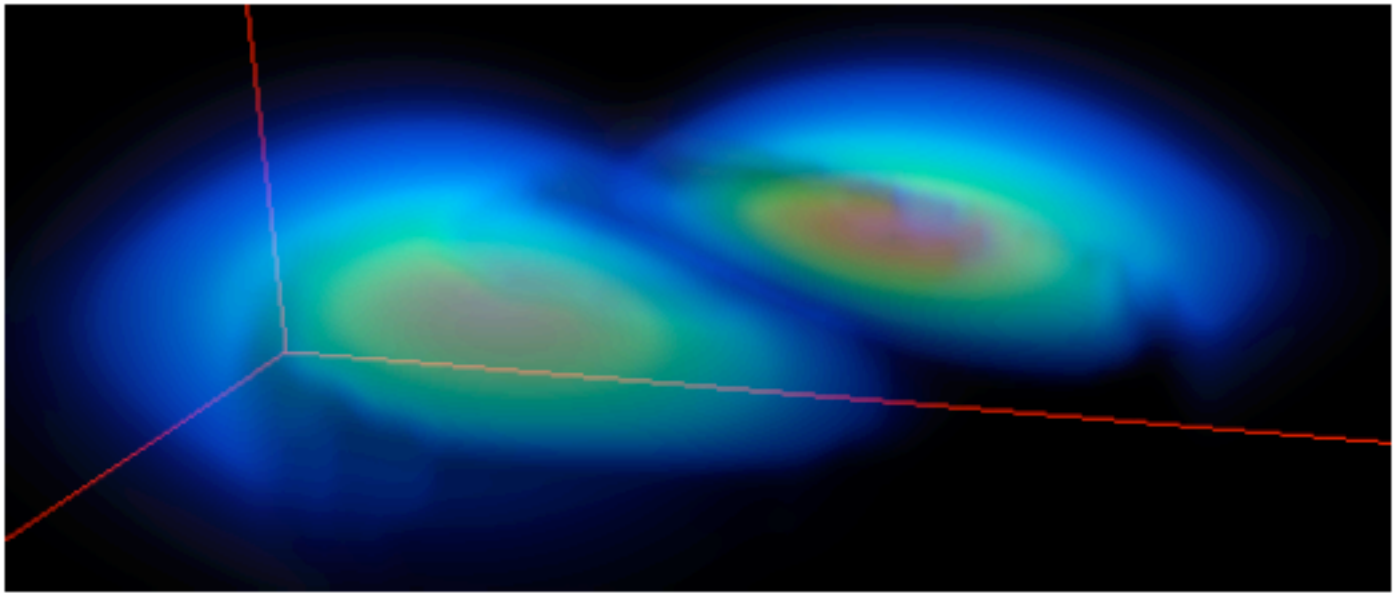
Result / Demonstrations / Impact:
- Visualization of 21 million atom wavefunction on single PC
- Interactive tool
- Analyze composition of wavefunction contributions
- Provided new physical insights

Authors:
- Wei Qiao (CS), David Ebert (ECE), Marek Korkusinski, Gerhard Klimeck



Publication was just accepted at premier IEEE Visualization conf.-88 of 268 accepted

VolQD
Drilling down into 3-D Volume Data



(a)

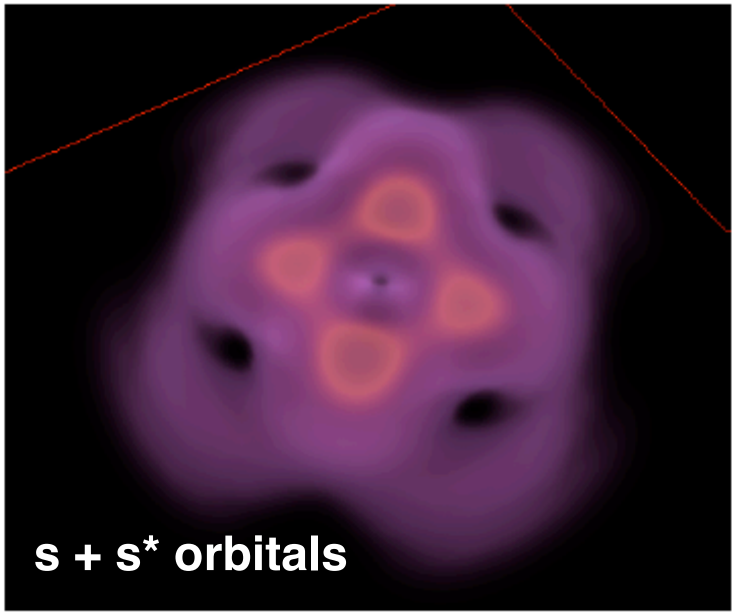
First excited state
(a) Volume data
(b-d) 2-D slices through data

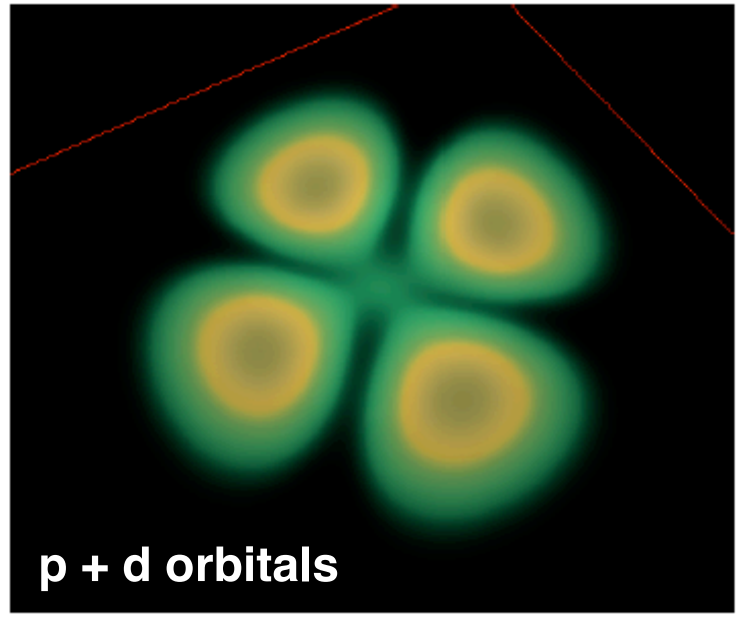
Statistical Analy:
Contributions in va...
orbitals vary spatially

Table 5: The percentage contributions of s, p, d and s* orbitals for the domains defined in Figure 12.

query domain	orbital contribution			
	s	p	d	s*
(a)	73.13%	1.08%	0.39%	25.68%
(b)	74.81%	0.64%	0.14%	24.42%
(c)	73.67%	0.98%	0.29%	25.07%
(d)	72.63%	1.13%	0.49%	25.76%

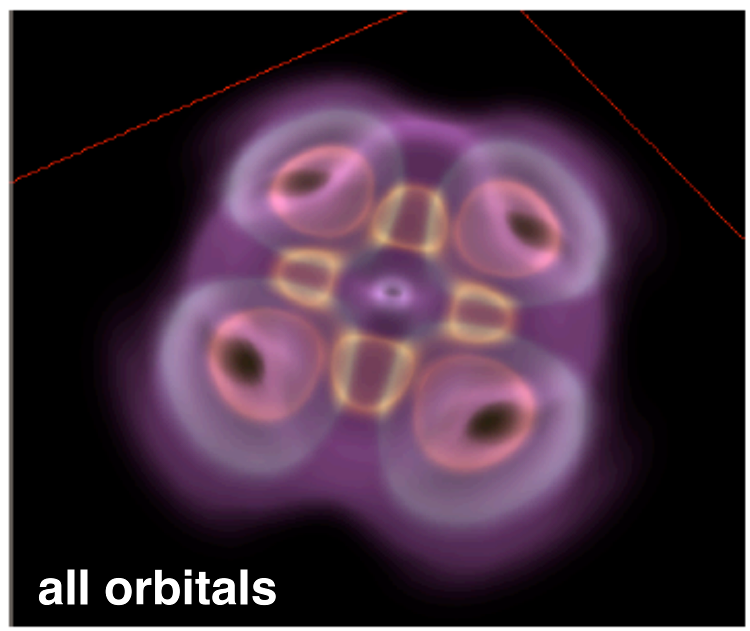
VolQD
Discovery of Surprising Nodal Symmetries





Second excited state
- Different orbital symmetries in (s+s*) versus (p+d)
- Discovery really enabled by visualization!

- Prompted additional investigations



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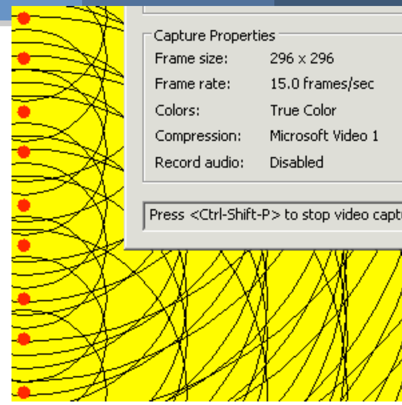
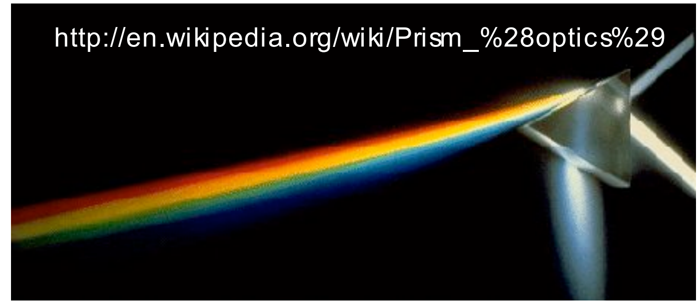
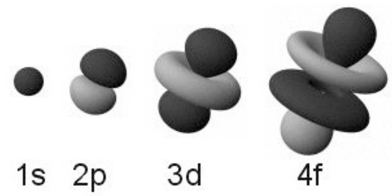
  - Particles
  - Propagating Waves
  - Standing Waves
  - Chromatography

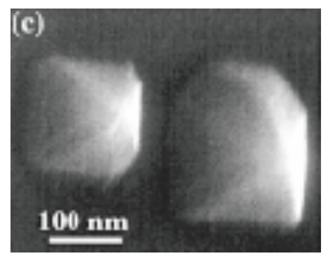




- Strange Experimental Results => The Advent of Quantum Mechanics
  - Discrete Optical Spectra
  - Photoelectric Effect
  - Particle-Wave Duality



- Quantum Dots
  - What is a Quantum Dot
  - Experimental Examples
  - Applications



- NEMO 3-D - Nanoelectronic Modeling
  - Multimillion Atom Simulations
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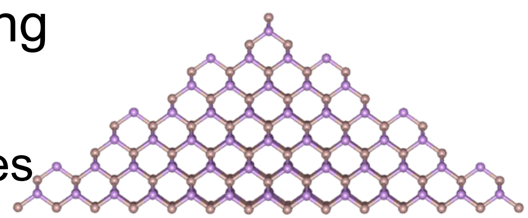
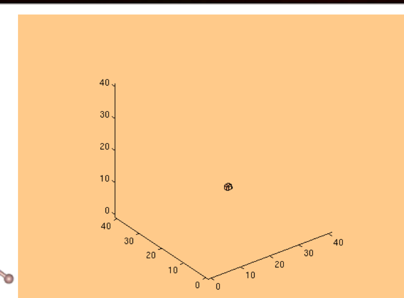
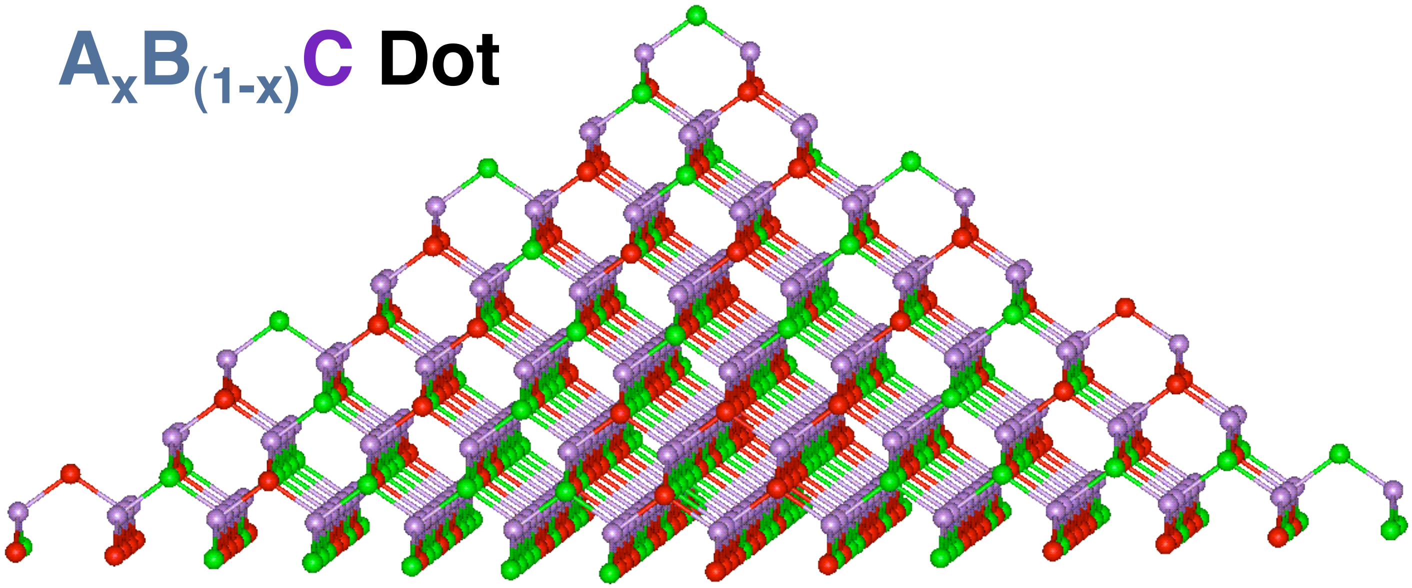




Alloy Disorder in Quantum Dots



- Compositional Alloys
  - Engineer dot size and energy spectrum
  - Engineer confinement potential
- Atomistic Simulation
  - Include disorder effects explicitly
  - Test validity of virtual crystal approximations