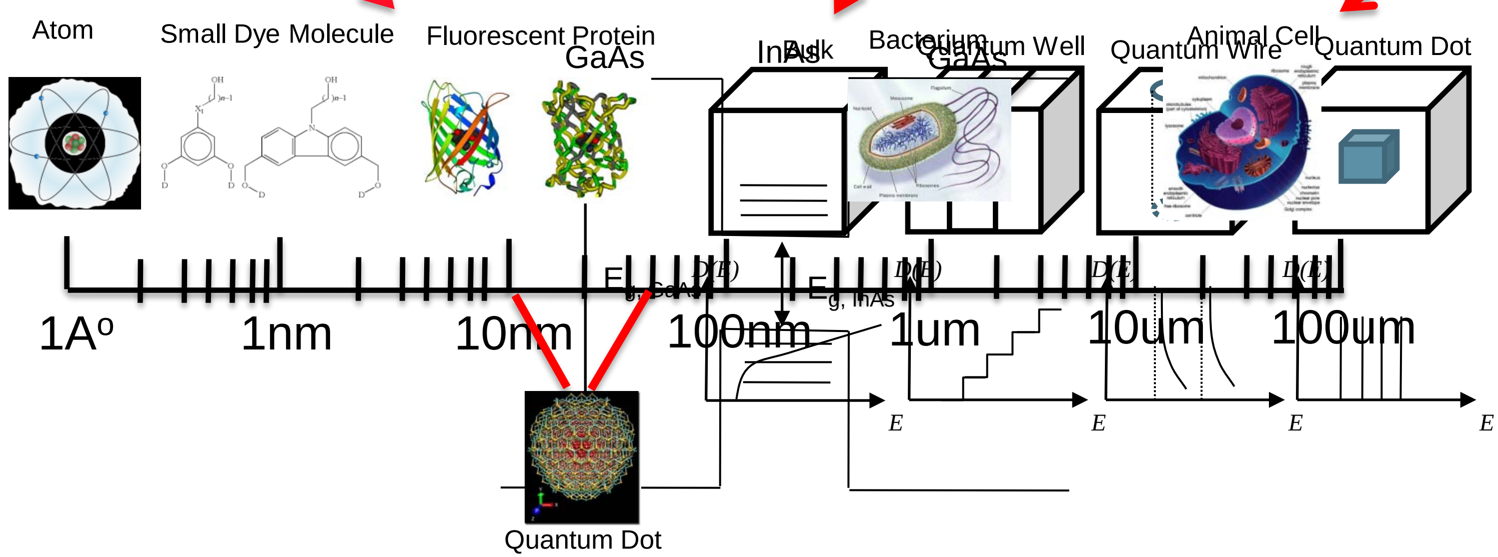
Introduction to Quantum Dots and Modeling Needs / Requirements

NCN

Gerhard Klimeck

What are Quantum Dots?

“Man-made nanoscale structure in which electrons can be confined in all 3 dimensions”



- ✓ Quantum Dots are larger than atoms
- ✓ 3-dimensional Confinement ➔ Discrete Energy levels ➔ “Artificial Atoms”
- ✓ Band gap Difference ➔ Low energy potential wells ➔ Hole and Electron Confinement

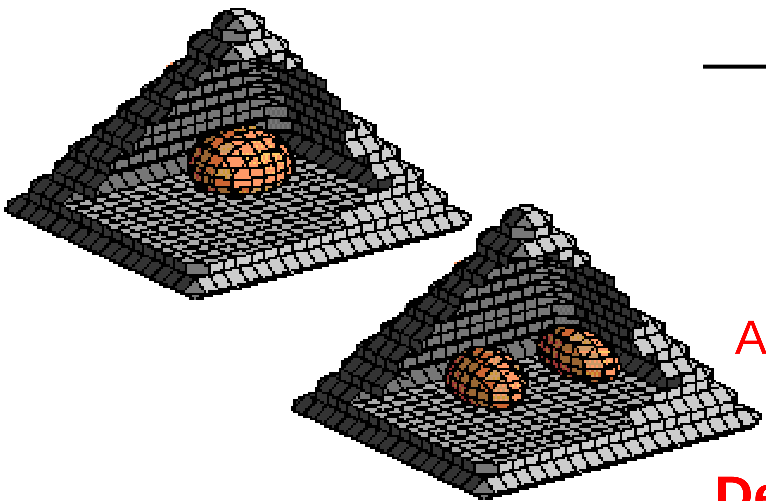
What is a Quantum Dot ? Basic Application Mechanisms

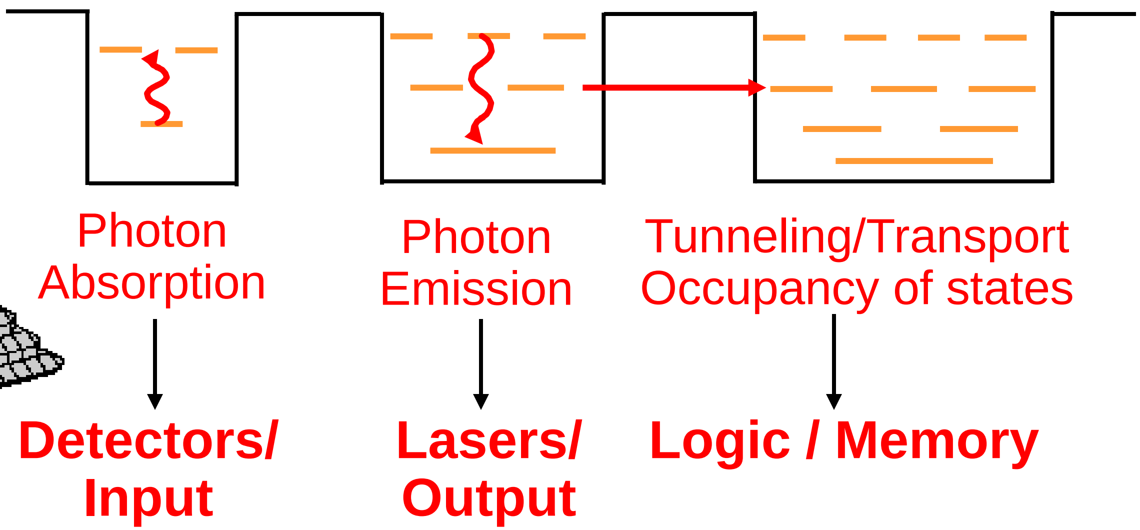
Physical Structure:

- **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:

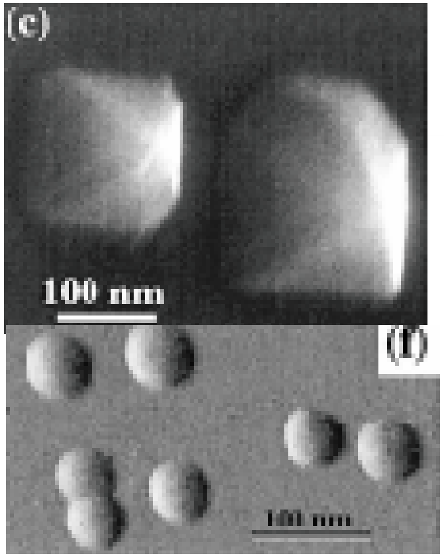
- **Electron energy may be quantized -> artificial atoms (coupled QD->molecule)**
- **Contains a countable number of electrons**





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

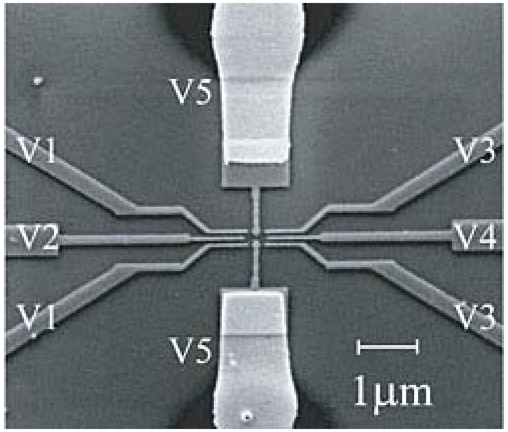
QD Example Implementations



Self-assembled ,
InGaAs on GaAs.

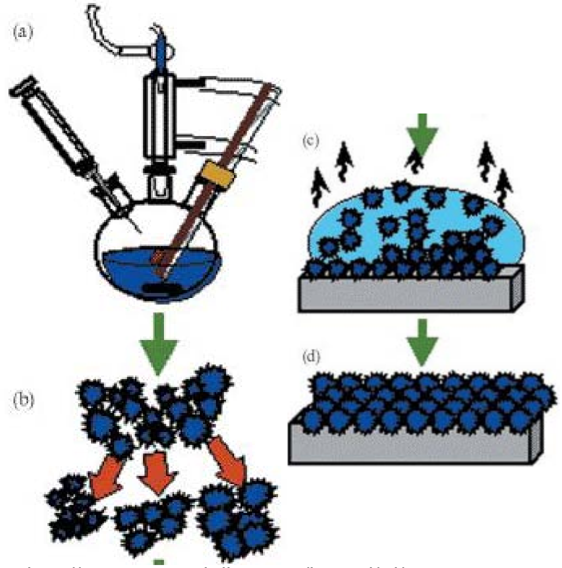
Pyramidal or dome shaped

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

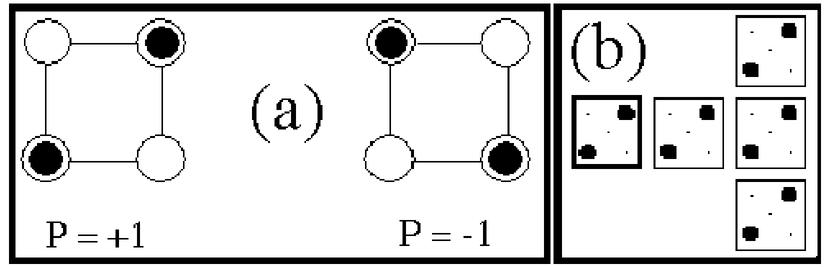
http://www.research.ibm.com/journal/rd/451

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

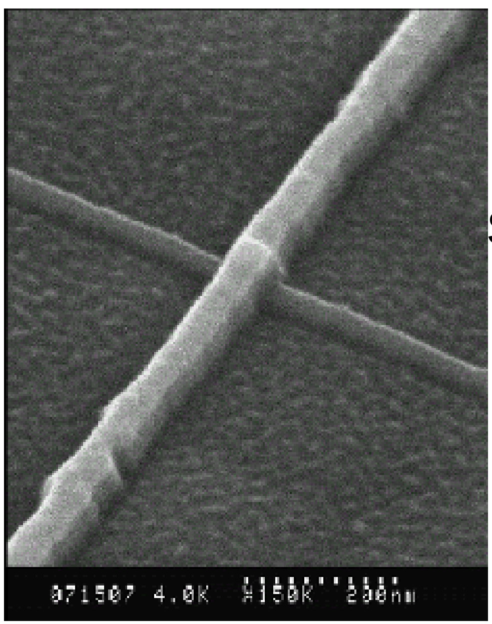
Source: http://en.wikipedia.org/wiki/Fluorescent ß

Quantum Dot Applications

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

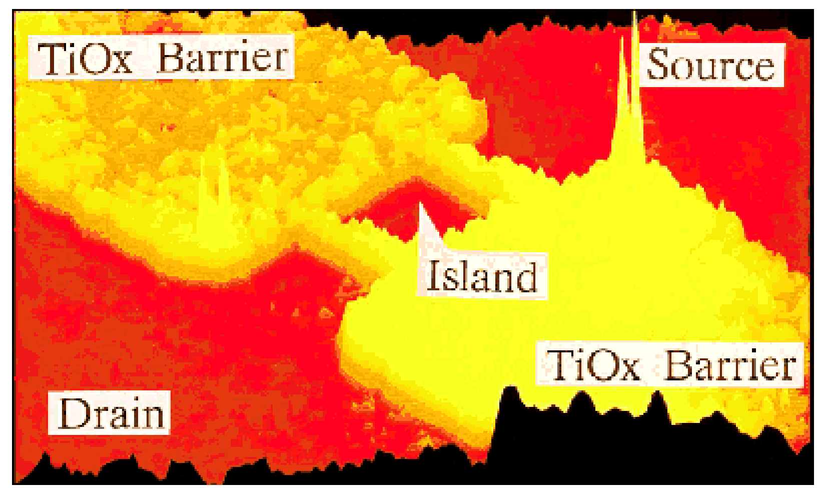


Lent, Porod @ Notre Dame: Quantum Cellular automata, electrostatically coupled quantum dots.



Chou @ Princeton
Room Temp.
Single Electron Memory

Hitachi:
128Mbit Integration demonstrated

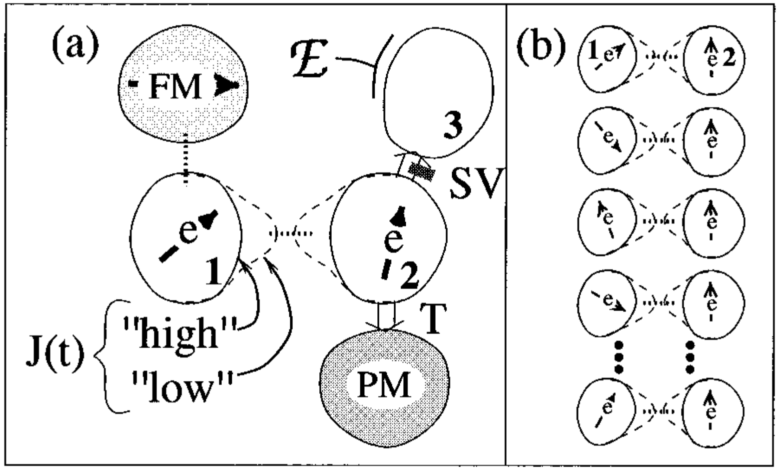


Harris @ Stanford: Room temperature single electron transistor

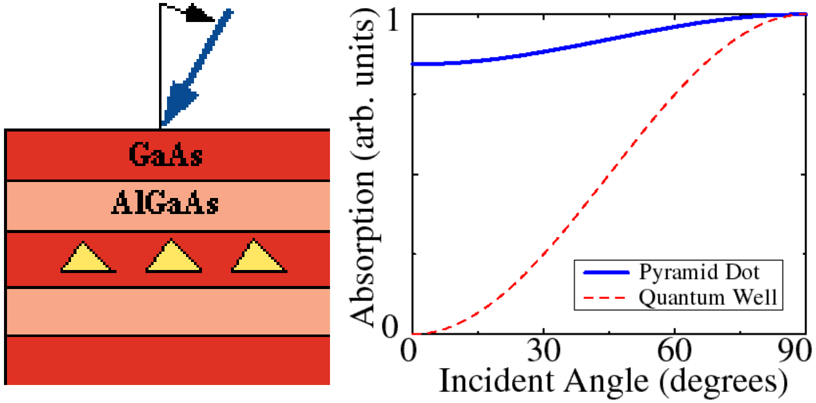
Quantum Dot Applications 2

- **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



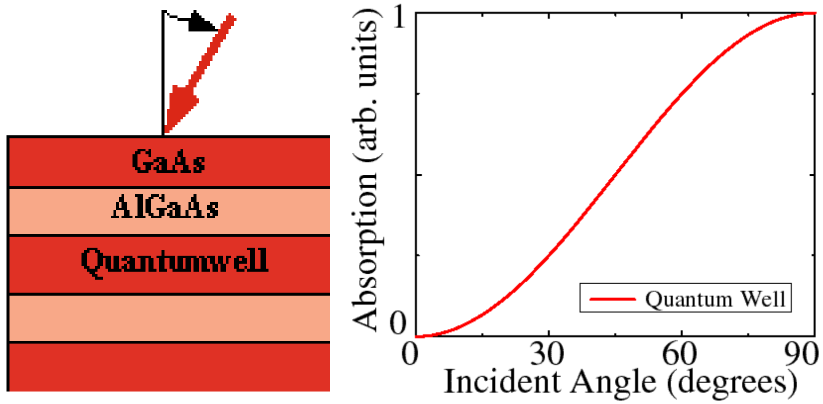
QDs for Quantum Computing



Quantum Dots: Absorption has weak incidence angle dependence

Quantum Dots as Optical Detectors

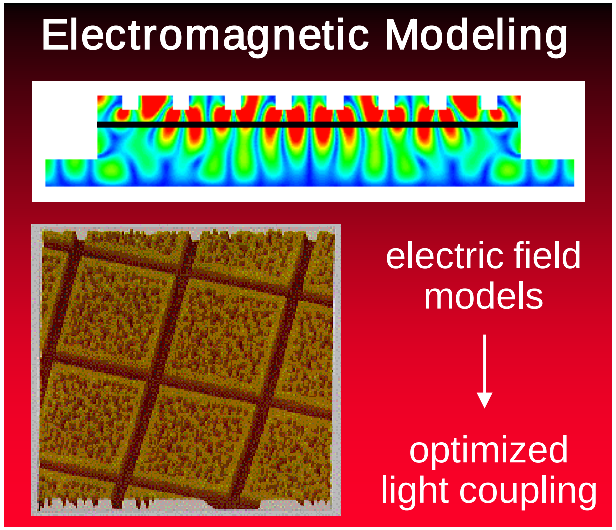
- **Problem:**
  Quantum wells are "blind" to light impinging orthogonal to the detector surface.
- **Standard Solution:**
  Need gratings to turn the light
- **New Approach:**
  Quantum dots have a built-in anisotropy and state quantization in all three dimensions
  -> absorption at all angles

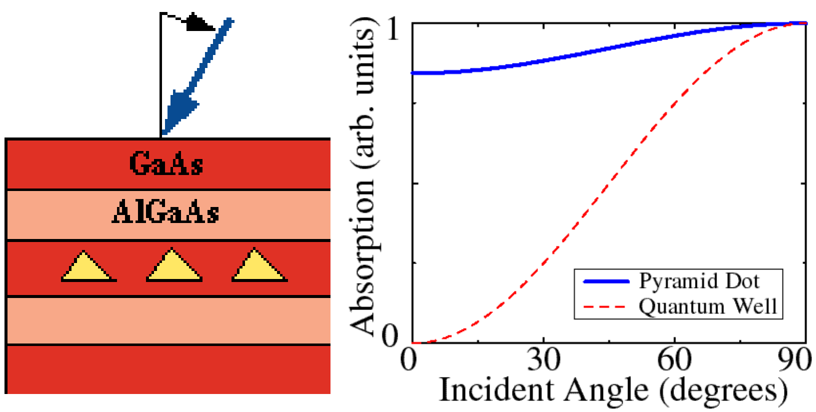


Quantum Wells: Absorption has strong incidence angle dependence

Standard Solution:

Grating





Quantum Dots: Absorption has weak incidence angle dependence

Lighting

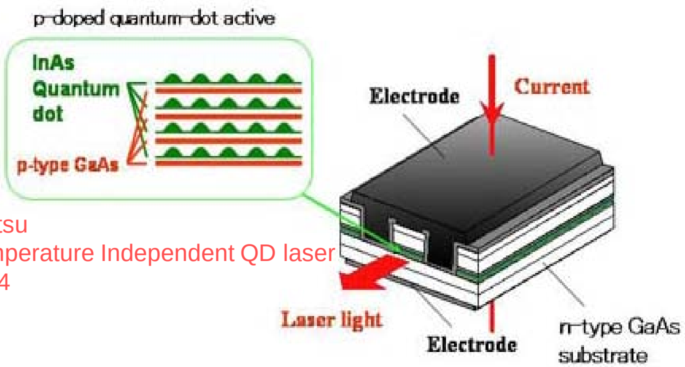
- Quantum-dot LEDs
  - » Seem to be key to advances in the fields of full-color, flat-panel displays and backlighting
- QD emits a color based on its size
  - » Smaller dots emit shorter wavelengths, such as blue, which, in the past, has been difficult to attain
  - » Larger dots emit longer wavelengths,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

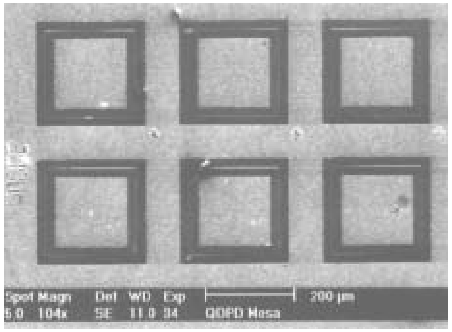
Some more Quantum Dot Applications

Room Temperature Lasers



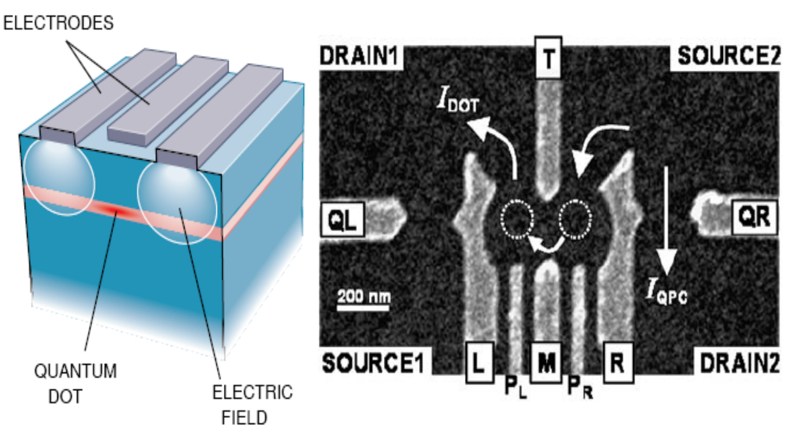
Fujitsu
Temperature Independent QD laser
2004

Infrared Photo-detector

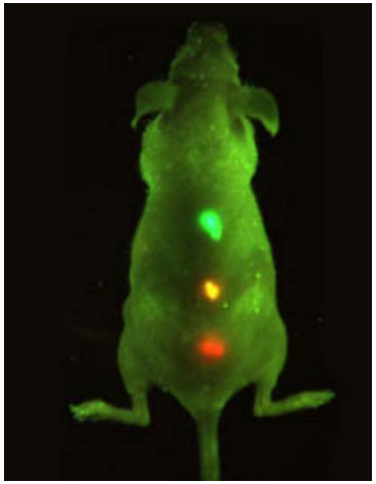


S. J. Xu
Dept. of Physics , University of Hong Kong (2005)

Quantum Gates



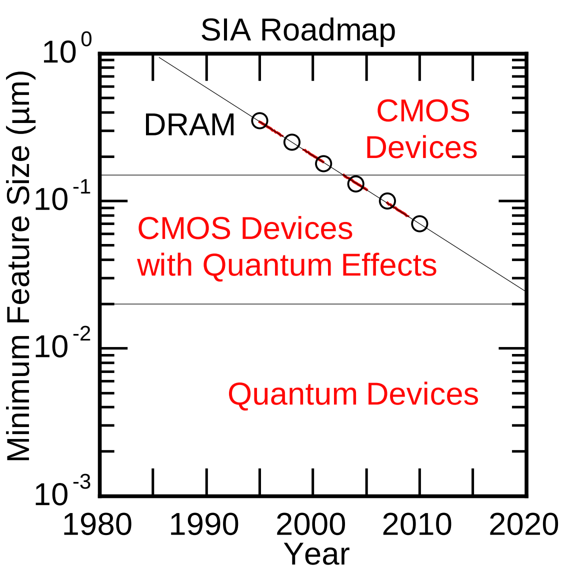
Quantum Dots Fluorescence Imaging

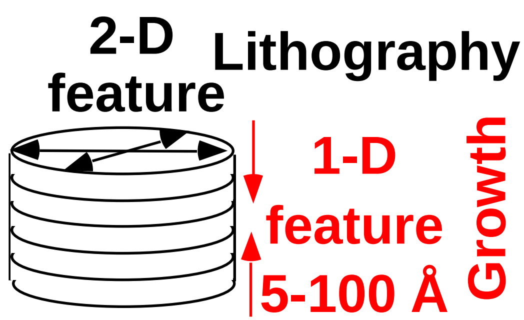


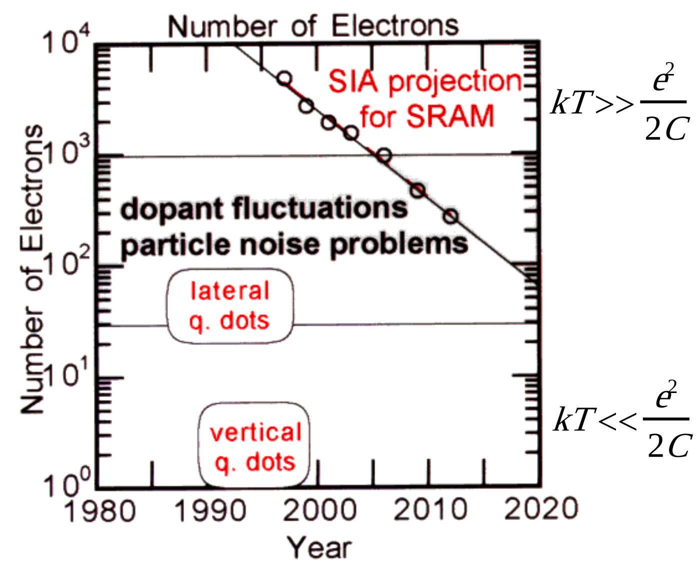
Sources: http://vortex.tn.tudelft.nl/grkouwen/qdotsite.html
http://www.whitaker.org/news/nie2.html

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





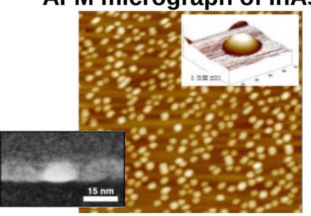


How can Quantum Dot Modeling Help?

- Why Theory, Modeling and Computation?

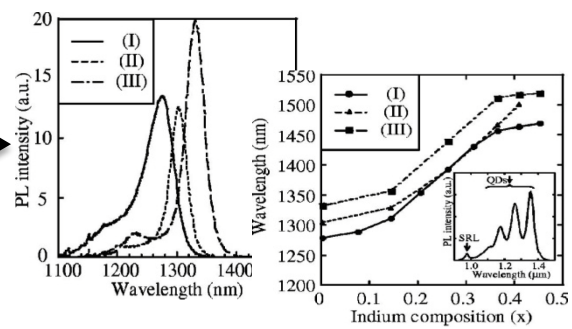
- Quantum dots grow in different shapes and sizes
- PL intensity is measured to determine light spectrum
- Experimentalists needs to understand the PL spectrum

AFM micrograph of InAs QD



Source: cqd.eecs.northwestern.edu/research/qdots.php

Missing Physics

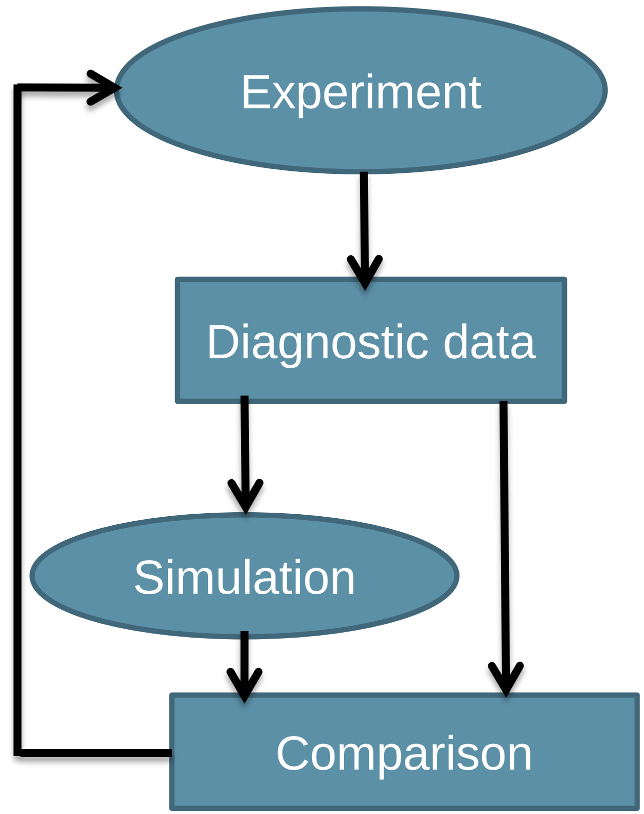


Applied Phys. Lett. 78, 3469 (2001)

✓ Modeling can provide essential insight into the physical data

✓ Obtain information where experimental data is not readily available

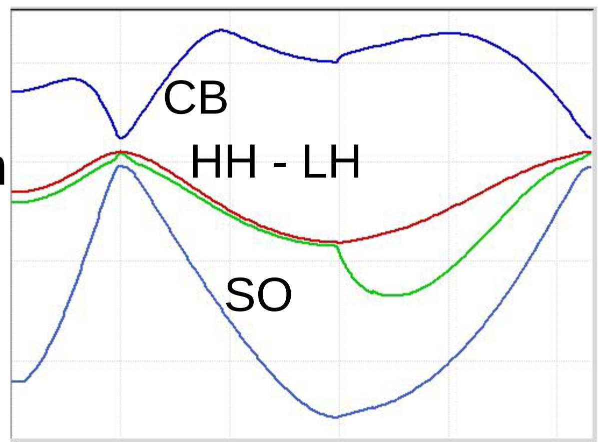
✓ Can help experimentalists to design their experiments

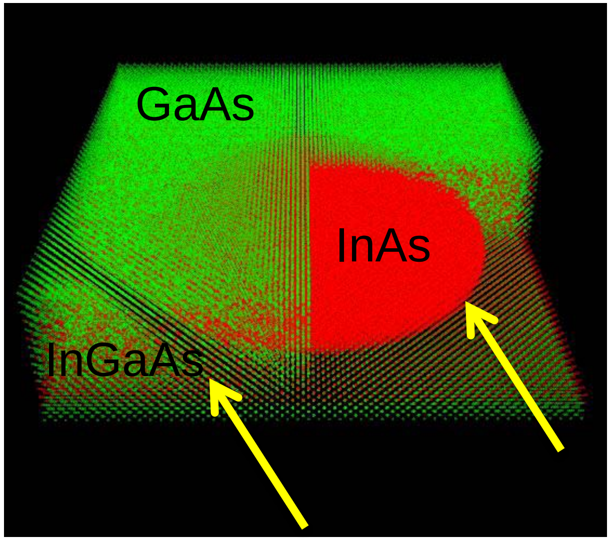


What is required in a good model for quantum dots?

- Realistic Size ➔ Strain domain ~ 10-15 million atoms, Electronic domain ~ 5-10 million atoms
- Interface roughness
- Alloy randomness
- Long range strain
- Non-parabolic dispersion
- Piezoelectricity

InAs bulk E(k) relation (www.nanoHUB.org)



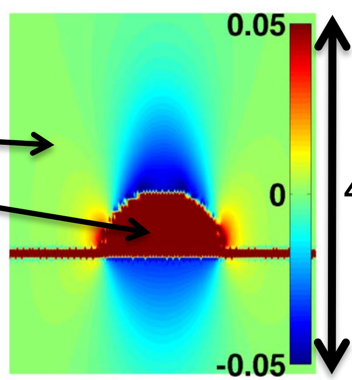


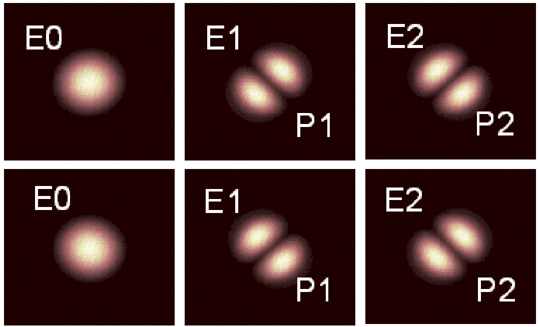
Acknowledgement: Insoo Woo (Purdue Univ)

Biaxial Strain

GaAs buffer

InAs Dome QD





Strain ➔ Yes
Piezo ➔ No

Strain ➔ Yes
Piezo ➔ Yes

Quantum dot modeling : What is out there ?(1)

✓Single-band Effective mass model

✓Multi-band Effective mass model
or
k•p method

✓Pseudo-potential Method

✓Tight Binding Model

Draw Back

- parabolic dispersion *E(k)* assumption.
- Ignore Interface roughness, alloy randomness
- Can not capture atomistic symmetry, optical anisotropy of p-states

Method

Individual Hamiltonians for electrons and holes:

$$H_e = -\frac{\hbar^2}{2m_e^*}\Delta + V_e(r) + E_g$$

$$H_h = -\frac{\hbar^2}{2m_h^*}\Delta + V_h(r)$$

m_e^* and m_h^* are effective masses

More bands can be added and couplings between the bands can be allowed (CB, HH, LH, SO).

8-band k•p method: coupling between conduction and valence bands

References:

1. D. Bimberg
2. C. Pryor
3. P. Hawrylak

O. Stier et *al*., PRB 59, 5688 (1999)
C. Pryor et *al*., PRB 57, 7190 (1998)

Quantum dot Modeling :What is out there? (2)

✓Single-band Effective mass model

✓Multi-band Effective mass model
or
k•p method

✓Pseudo-potential Method

✓Tight Binding Model

Draw Back

- Computationally expensive

➔ Hard to simulate realistic device sizes

Method

- Potential of ions and core electrons is replaced by "pseudopotential".
- Plane wave basis states:

$$H_{pp} = -\frac{\hbar^2}{2m}\Delta + \sum_i V_{pp}(r - R_i)$$

$$\psi_{pp} = \sum_k c_k e^{ikr}$$

Pseudopotential is decided atomistically on the basis of atom locations ➔ Atomistic representation

References:

1. Alex Zunger

A. Zunger, Phys. Status Solidi B 224, 727 (2001)

Quantum dot modeling : what is out there? (3)

- ✓Single-band Effective mass model
- ✓Multi-band Effective mass model
  or
  k•p method
- ✓Pseudo-potential Method
- ✓Tight Binding Model

<u>Why Tight Binding?</u>

- Atomistic details
- Computationally less expensive
- Correct band mixing
- Band structure over entire Brillouin zone

Hamiltonian in terms of linear combination of atomic orbitals:

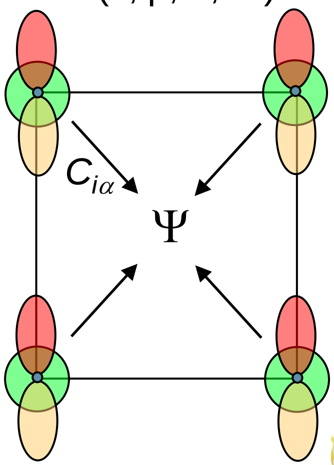
$$\psi(\mathbf{r}) = \sum_{\substack{\text{atomic} \\ \text{site, } i}} \sum_{\text{orbitals, } \alpha} C_{i\alpha}\, \phi_{i\alpha}(\mathbf{r} + \mathbf{R}_i)$$

$C_{i\alpha}$= coefficients, $\phi_{i\alpha}$= atomic orbitals (s, p, d, s*)

$$H_{i\alpha,j\beta} = \langle \phi_{i\alpha} | H | \phi_{j\beta} \rangle = \langle i\alpha | H | j\beta \rangle = \int d\mathbf{r}\, \phi^*_\beta (r - R_j) H \phi_\alpha (r - R_i)$$

On-site and coupling matrix elements are calculated empirically by matching experimentally found band gaps, effective masses etc

ϕ= orbital(s, p, d, s*)



<u>Reference:</u>

1. Boykin, Klimeck
2. Jean-Marc Jancu

G. Klimeck et *al*., CMES (2004), Vol.3 no. 5, pp601-642