Development of a 3-D Nanoelectronic Modeling Tool NEMO-3D

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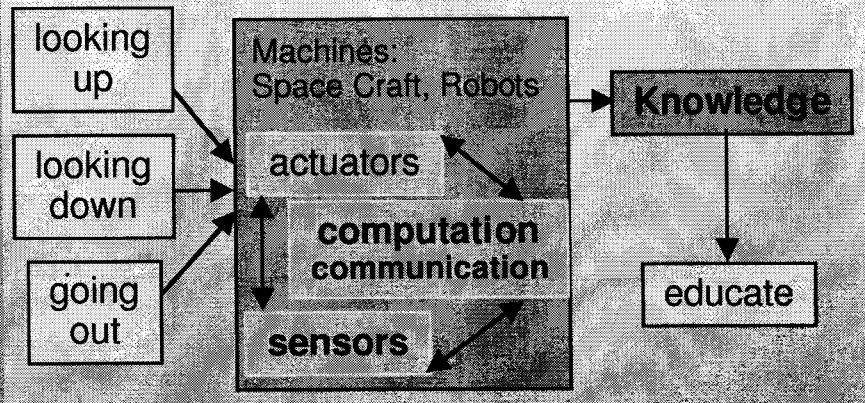
Revolutionary Computing and Sensing are Enabled by Nanoelectronics

4 Basic NASA Missions: Enabled by Technology



Example NASA Mission Requirements:
- Autonomous spacecraft
- In-situ data analysis
- On-board image processing

=> Beyond existing system technology

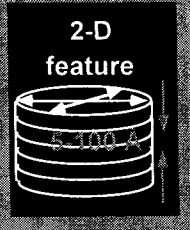
Device/System Requirements:
- Low power and weight, however massive computing and sensing
- Radiation hard devices

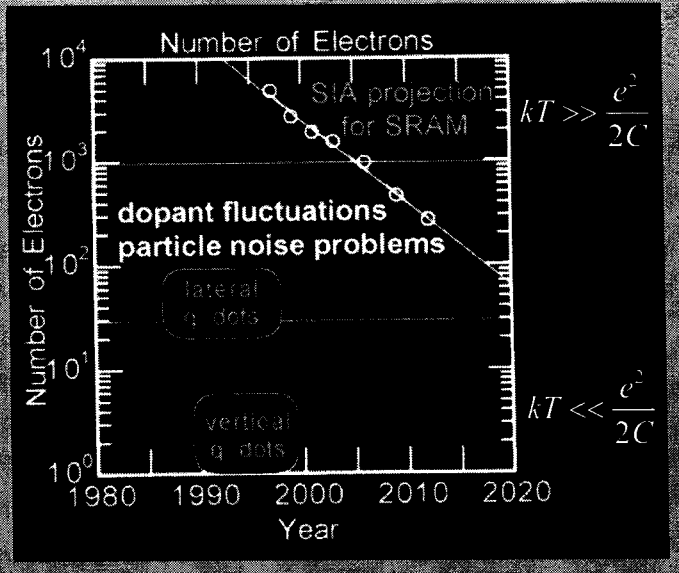
=> Beyond existing device technology

Nanoelectronics:
- Don't fight, **utilize** quantum behavior:
  - Quantized charge
  - Quantized energy
- Artificial Atoms & Molecules
- Custom optical transitions
- New computation architectures

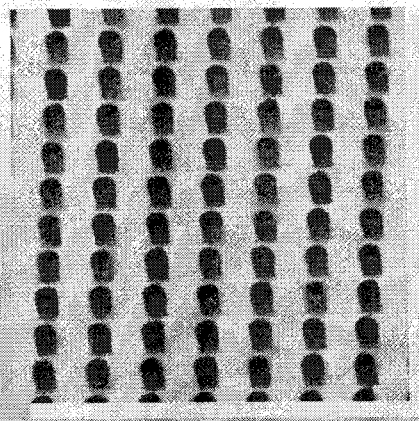
=> Bottom-up 3-D, atomistic device simulation

Another Look at Moore's Law



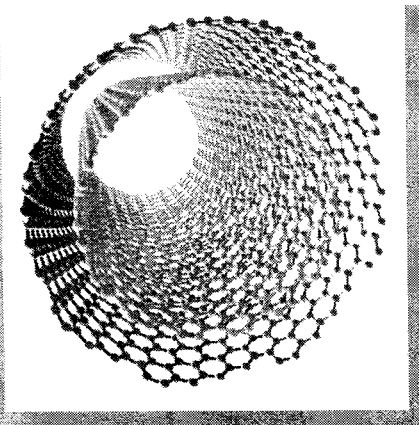


Examples of 3D Confined Structures



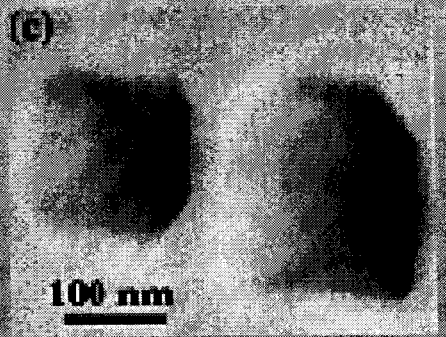
Quantum Dots:
Litho-based,
GaAs/AlGaAs,
InGaAs/InAlAs
systems

Cylinder shaped
M Reed et al, TI
(1988)



Fullerenes, C60:
Carbon based
Electronic and
mechanical appl.

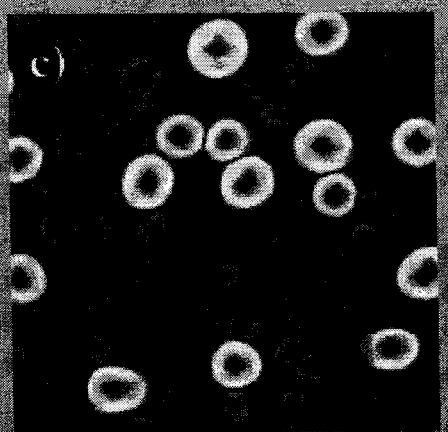
Rice Univ.,
NASA Ames



Quantum Dots:
Self-assembled ,
InAs on GaAs.

Pyramidal or
dome
shaped

R. Leon et al,
JPL (1998)

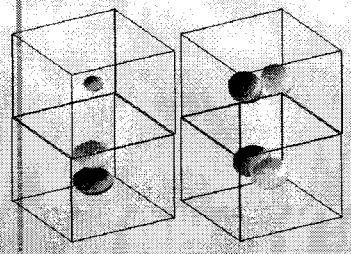


Quantum Dots:
Self-assembled ,
Ge on Si.

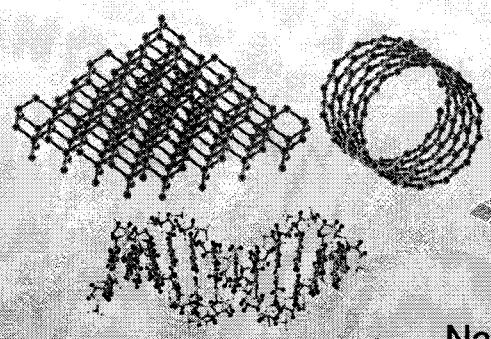
Dome
shaped

S. Williams et al,
HP (1998)

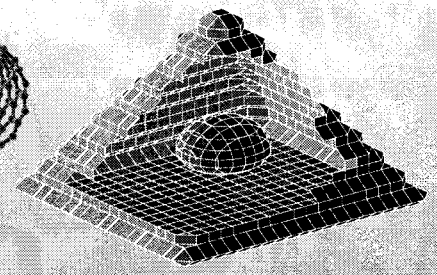
Quantum Dot Simulation for Revolutionary Computing and Sensing



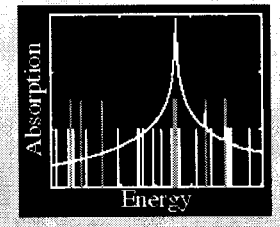
Atomic Orbitals
size: 0.2nm



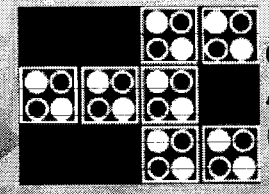
Structure



Nanoscale Quantum States
(Artificial Atoms, size 20nm)



Designed
Optical
Transitions
Sensors



Quantum Dot
Arrays
Computing

Opportunity:

- Nanoscale electronic structures can be built!
  => Artificial Atoms / Molecules

Problem:

- The design space is huge: choice of materials, compositions, doping, size, shape.

Approach:

- Deliver a 3-D atomistic simulation tool
- Enable analysis of arbitrary crystal structures, atom compositions and bond/structure configurations.

NASA Relevance:

- 2-5μm Lasers and detectors
- High density, low power computation (logic and memory)
- Life signature biosensors

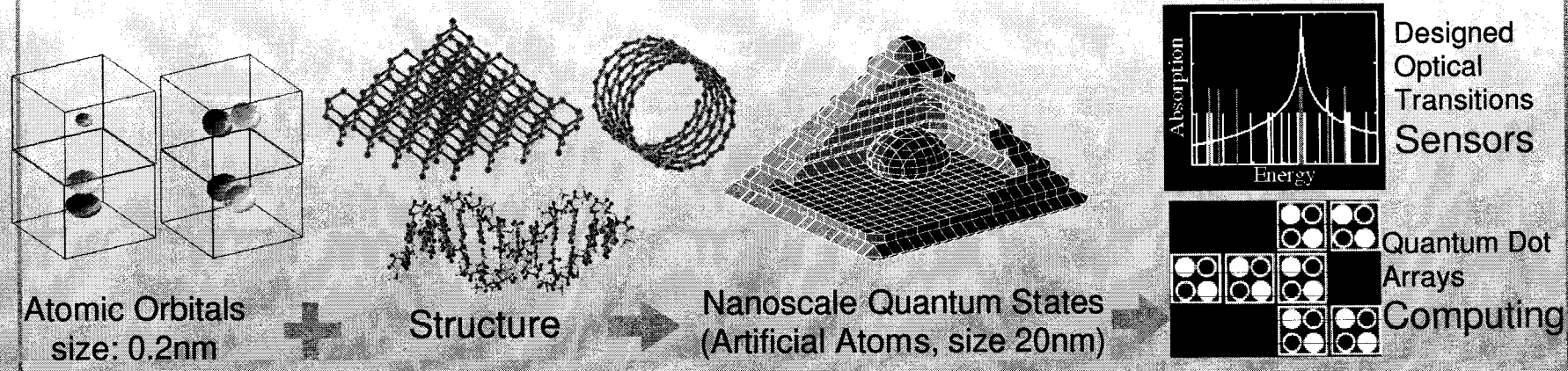
Impact:

- Low cost development of revolutionary technology.
- Narrow empirical/experimental search space

Collaborators:

- Ames, University of Alabama-Huntsville, Purdue

Quantum Dot Simulation for Revolutionary Computing and Sensing



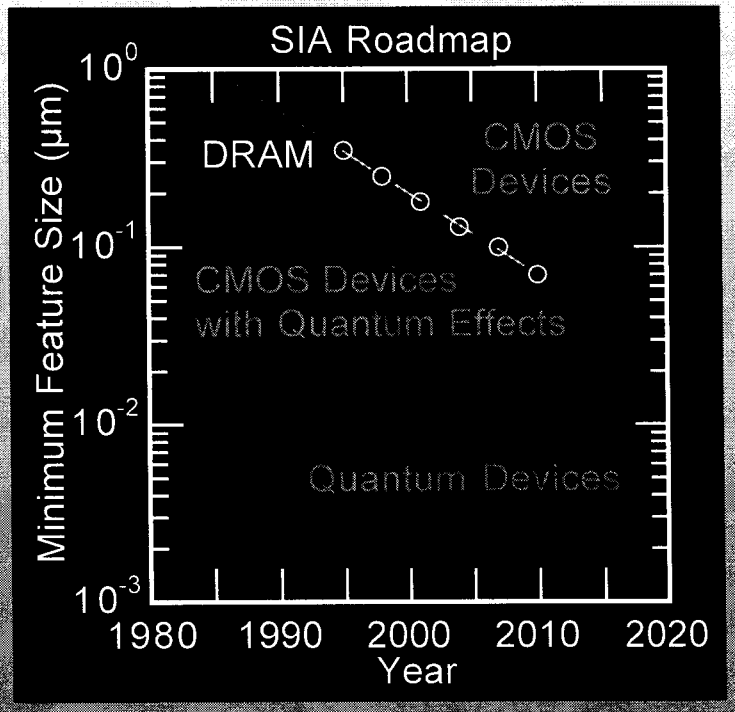
Outline:

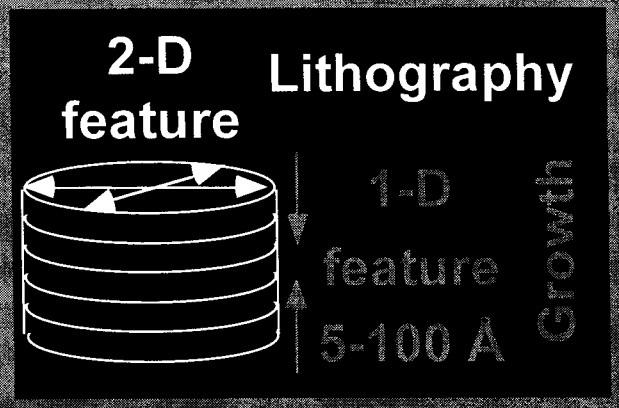
- NEMO - 1D : Heterostructures: what are they? how do you engineer them?
- Mapping of orbitals to semiconductor band structure (genetic algorithm fitting)
- Strain in self-assembled quantum dots
- Computation of nanoscale quantum states - artificial atomic states
- Optical Transitions in Quantum Dots
- Quantum dot computing presented earlier in the day by Amir Fijany
- How do you know what you built?
  Non-invasive device characterization by simulation.
- Software Structure
- Teaser on: THz response, Hole Transport, and Bandstructure models
- Future Outlook

Leverage Nanoelectronic Modeling (NEMO)

- **NEMO was developed under a government contract to Texas Instruments and Raytheon from 1993-1997**
  - **>50,000 person hours of research and development**
  - **250,000 lines of code in C, FORTRAN and F90**
  - Theory
    - Roger Lake, Chris Bowen, Gerhard Klimeck, Tim Boykin (UAH)
  - Graphical User Interface
    - Dan Blanks, Gerhard Klimeck
  - Programming Approach, Philosophy, and Prototypes
    - Bill Frensley (UTD), Gerhard Klimeck, Chris Bowen
  - Coding Help
    - Manhua Leng (UTD), Chenjing Fernando, Paul Sotirelis, Dejan Jovanovic, Mukund Swaminathan (UTA),
  - Experiments for verification
    - Ted Moise, Alan Seabaugh, Tom Broekaert, Berinder Brar, Yung-Chung Kao
- **Gerhard Klimeck and Chris Bowen were the core developers.**
- **NEMO in THE state-of-the-art heterostructure design tool.**
- **Used at Intel, Motorola, HP, Texas Instruments, and >10 Universities.**

Microdevices Head for Atomic Dimensions



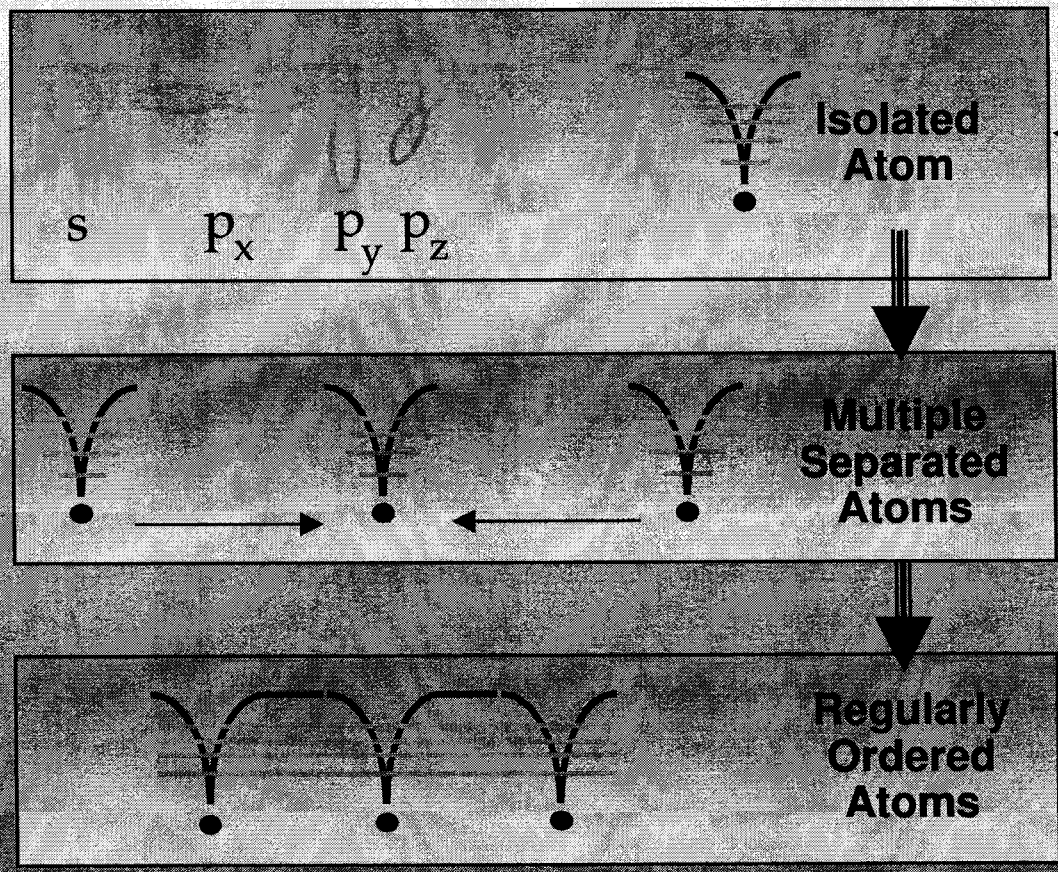


- **Moore's Law shows quantum devices in the far future.**
- **Lithography data alone is deceiving:** Layer thicknesses are already on the atomic length scale!
- **Commercial devices see quantum limitations:**
  - **direct tunneling**
  - **state quantization**
- **Advanced devices utilize the quantum mechanical behavior:**
  - **Resonators (RTDs)**
  - **Active and passive sensors tunable by design - not by material system choice (QWIP).**

-> 1D quantum device modeling

-> NEMO

Bandstructure Basics
Electron Conduction in Solids



Gas

Quantum Mechanics
Optical Transitions
Coulomb Repulsion

Physics

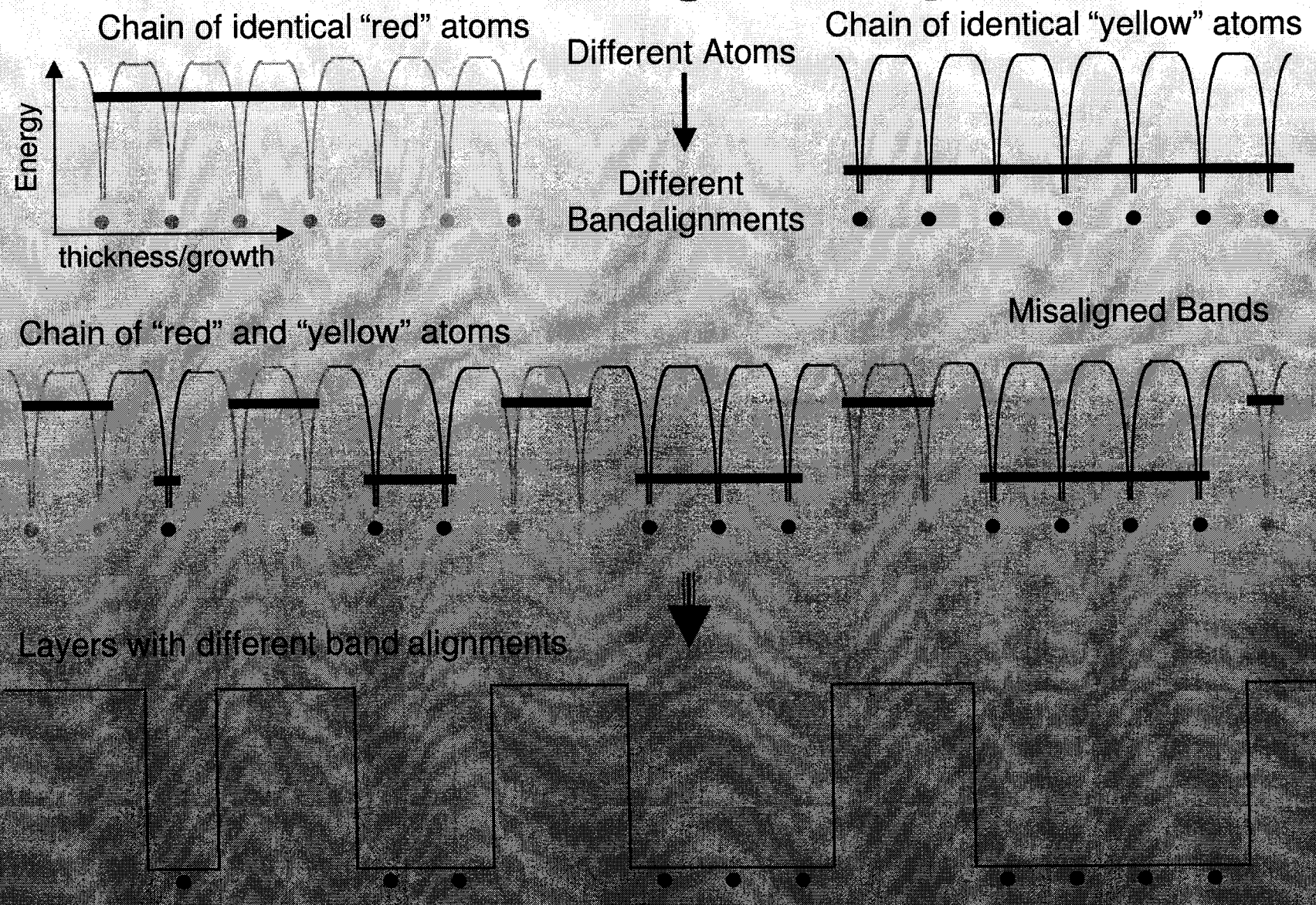
Solid

Transport
conductivity, mobility

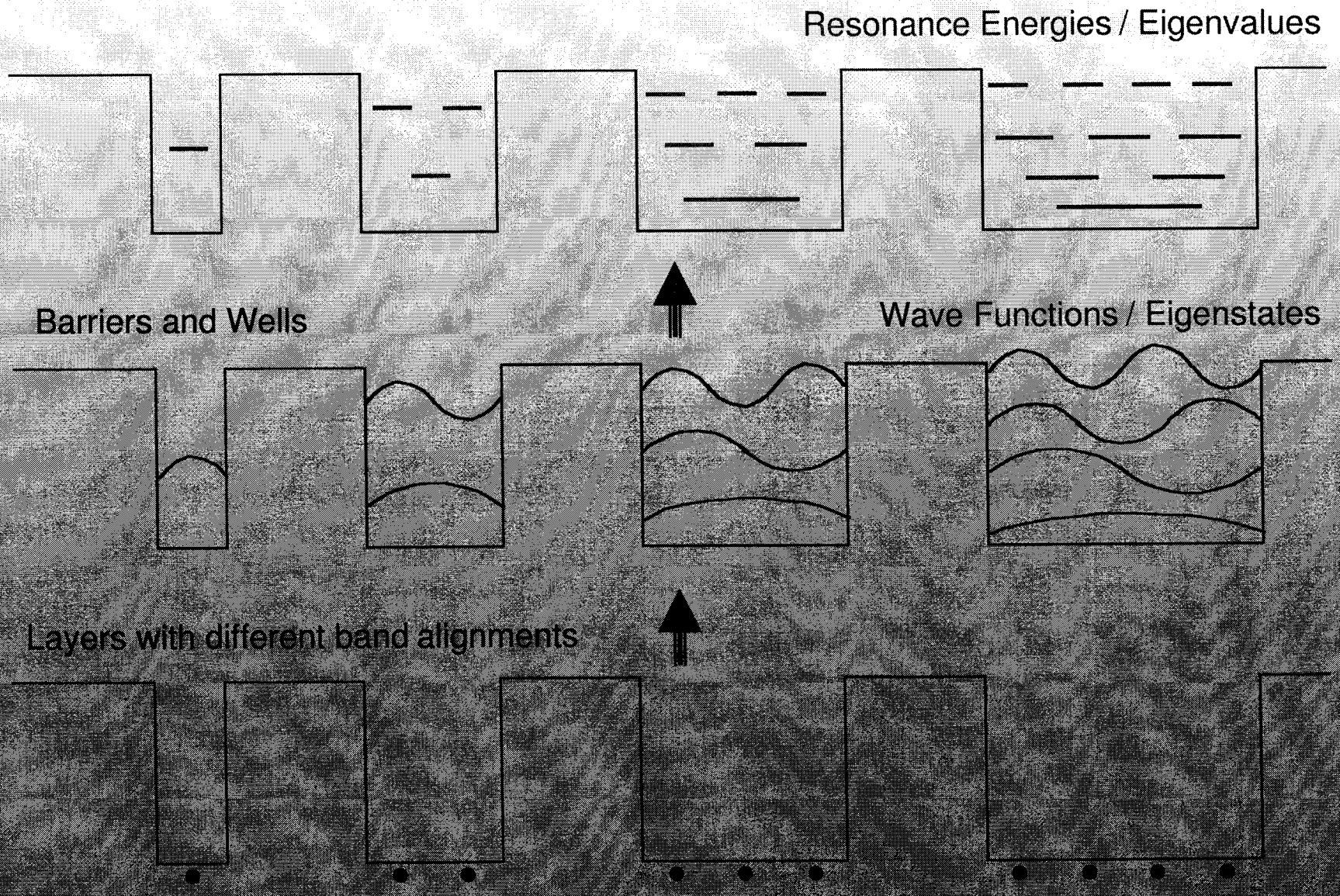
Devices

- Bands are channels in which electrons move "freely".
- Layers of **different** atoms are deposited with **monolayer** control.
- We can **engineer** the electron **bands**.

Bandstructure Engineering Basics

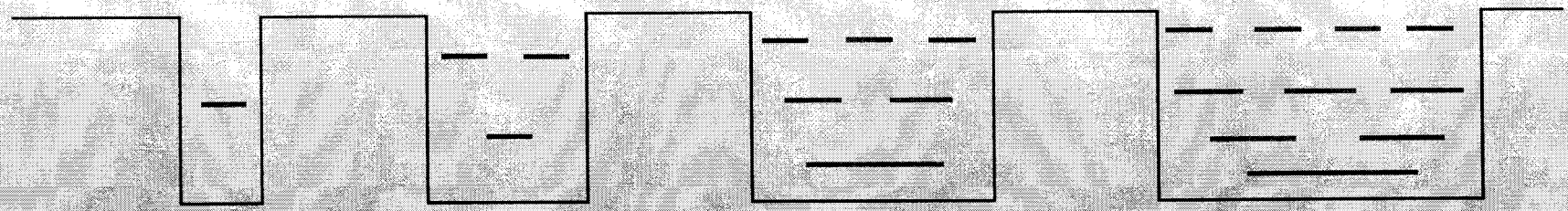


Bandstructure Engineering Basics



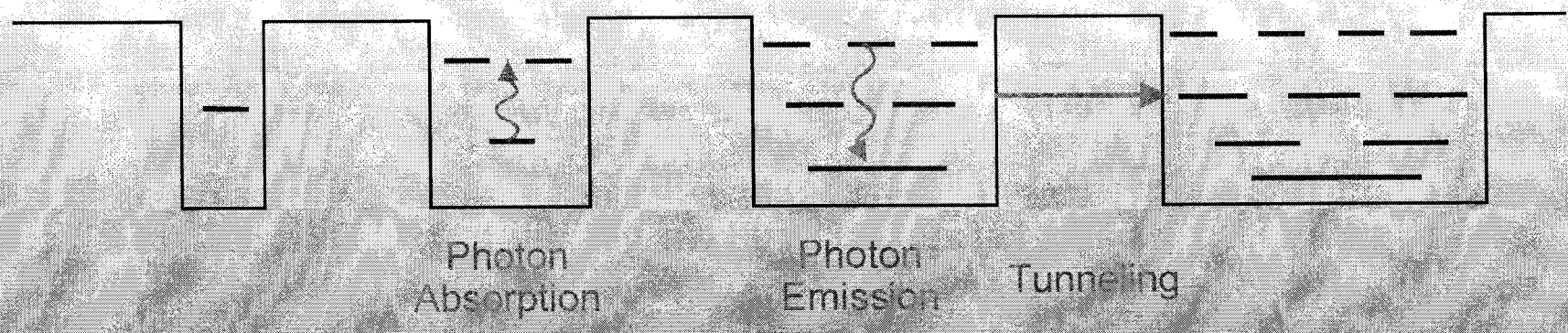
Bandstructure Engineering Basics

Resonance Energies / Eigenvalues



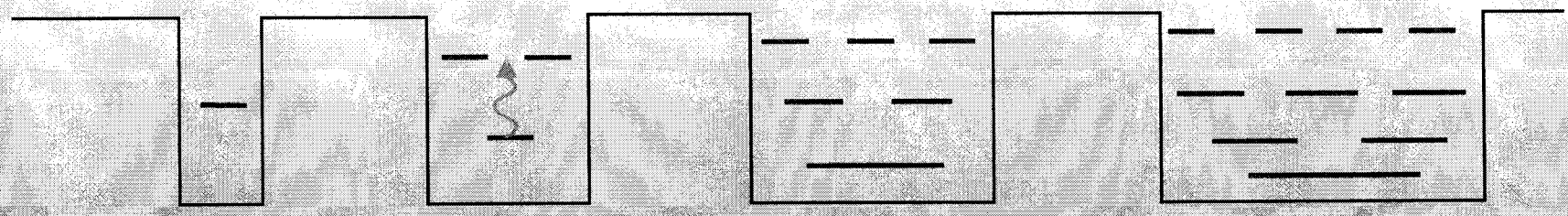
Bandstructure Engineering Applications

Transitions / Transport



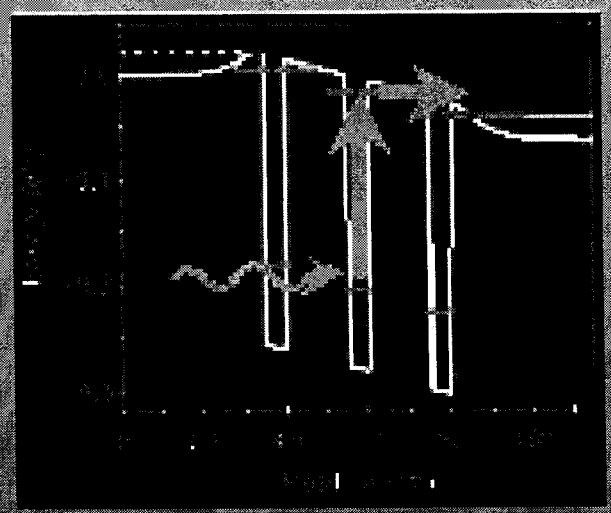
Bandstructure Engineering Applications

Transitions / Transport



Photon Absorption

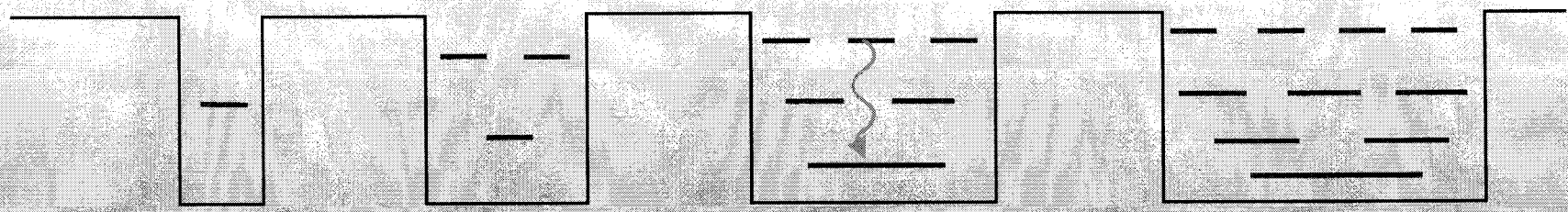
Detectors



Quantum Well Infrared Detector

Bandstructure Engineering Applications

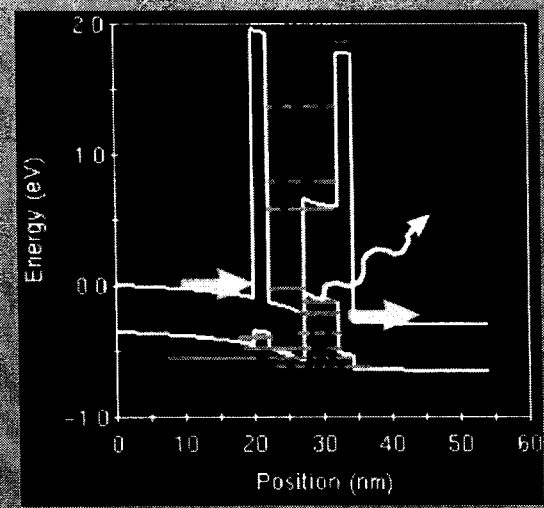
Transitions / Transport



Photon Emission

↓

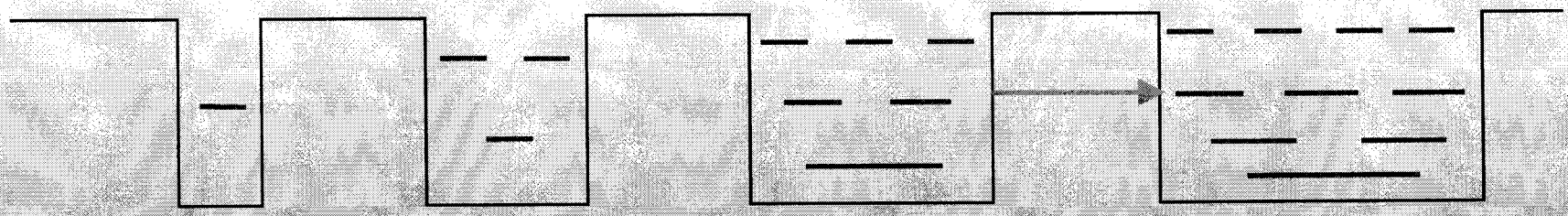
Lasers



Quantum Cascade Laser

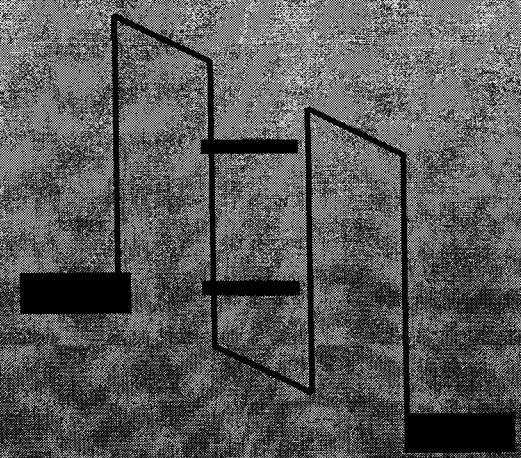
Bandstructure Engineering Applications

Transitions / Transport



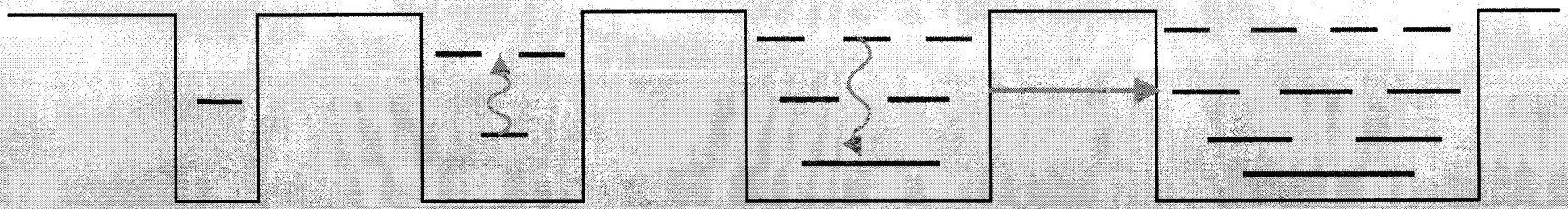
Tunneling

Logic / Memory

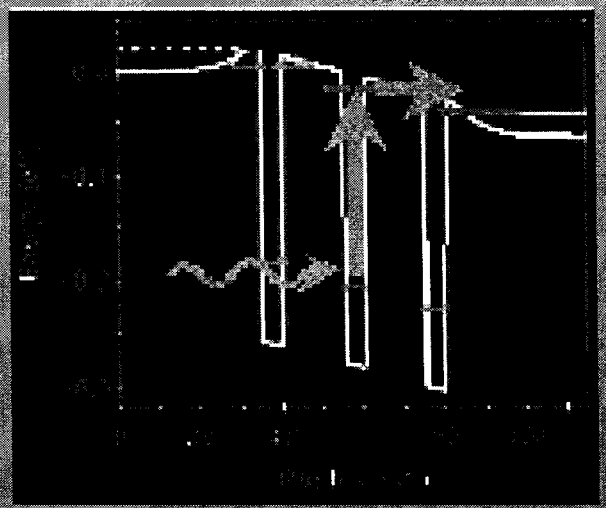


Resonant Tunneling Diode

Transitions / Transport Controlled by Design

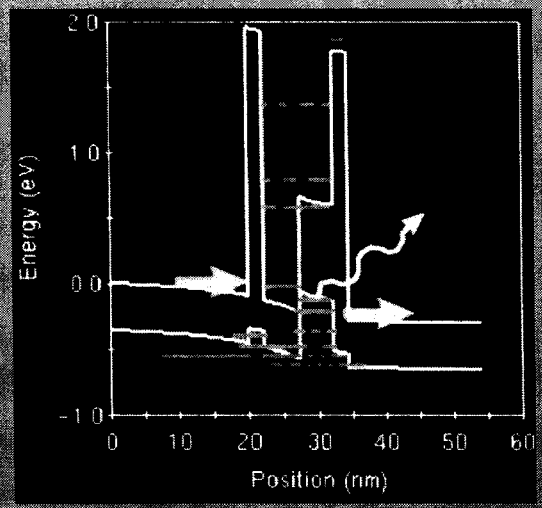


Detectors



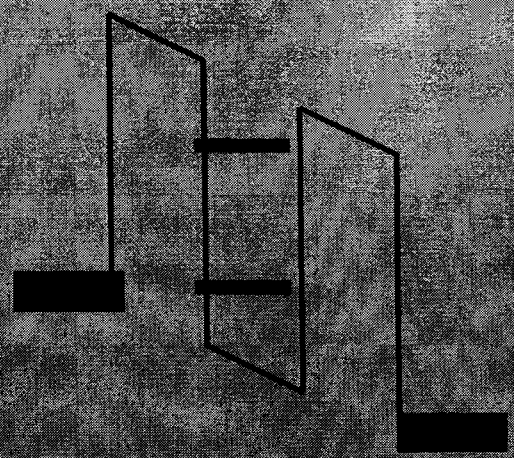
Quantum Well
Infrared Detector

Lasers



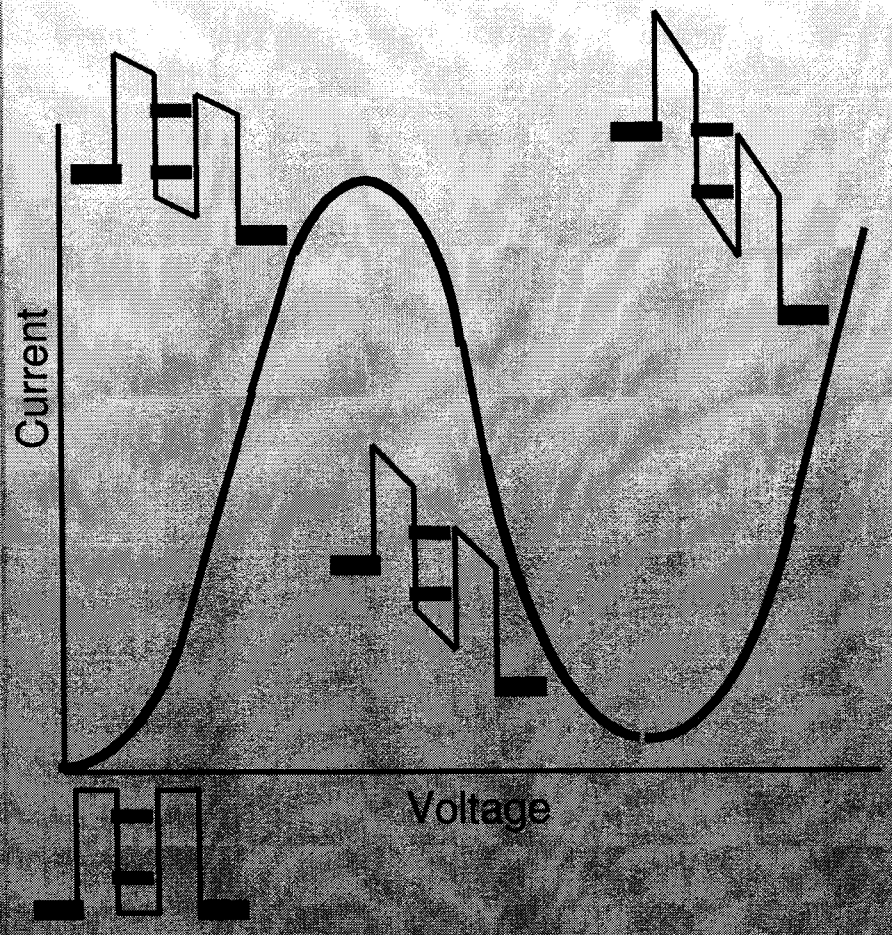
Quantum Cascade
Laser

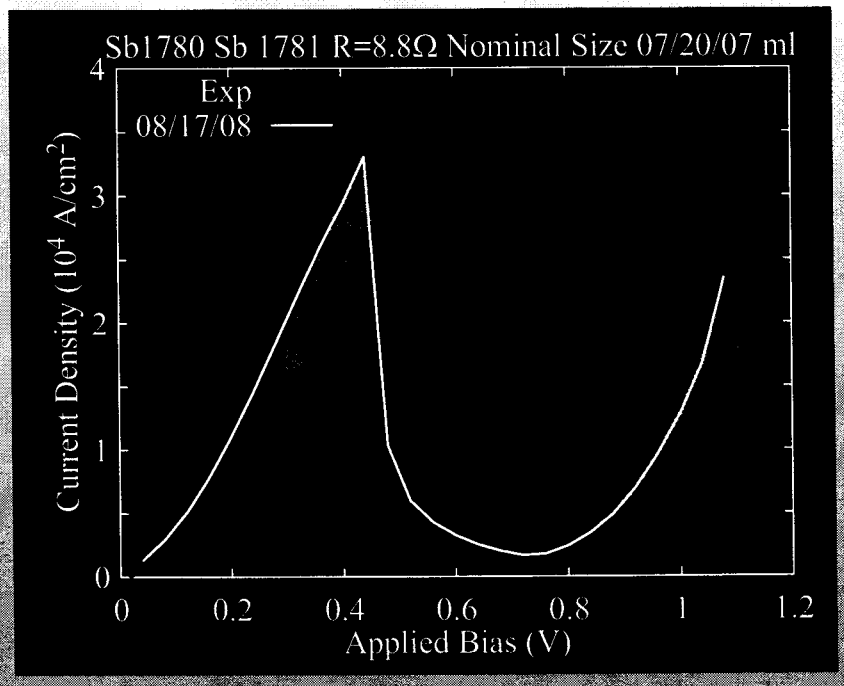
Logic / Memory



Resonant
Tunneling
Diode

Resonant Tunneling Diode





12 different I-V curves: 2 wafers, 3 mesa sizes, 2 bias directions

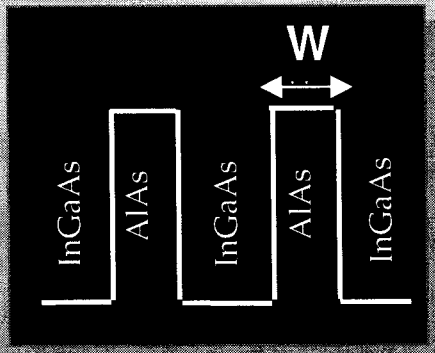
50nm	1e18	InGaAs
7 ml	nid	InGaAs
7 ml	nid	AlAs
20 ml	nid	InGaAs
7 ml	nid	AlAs
7 ml	nid	InGaAs
50 nm	1e18	InGaAs

Conduction band diagrams for different voltages and the resulting current flow.

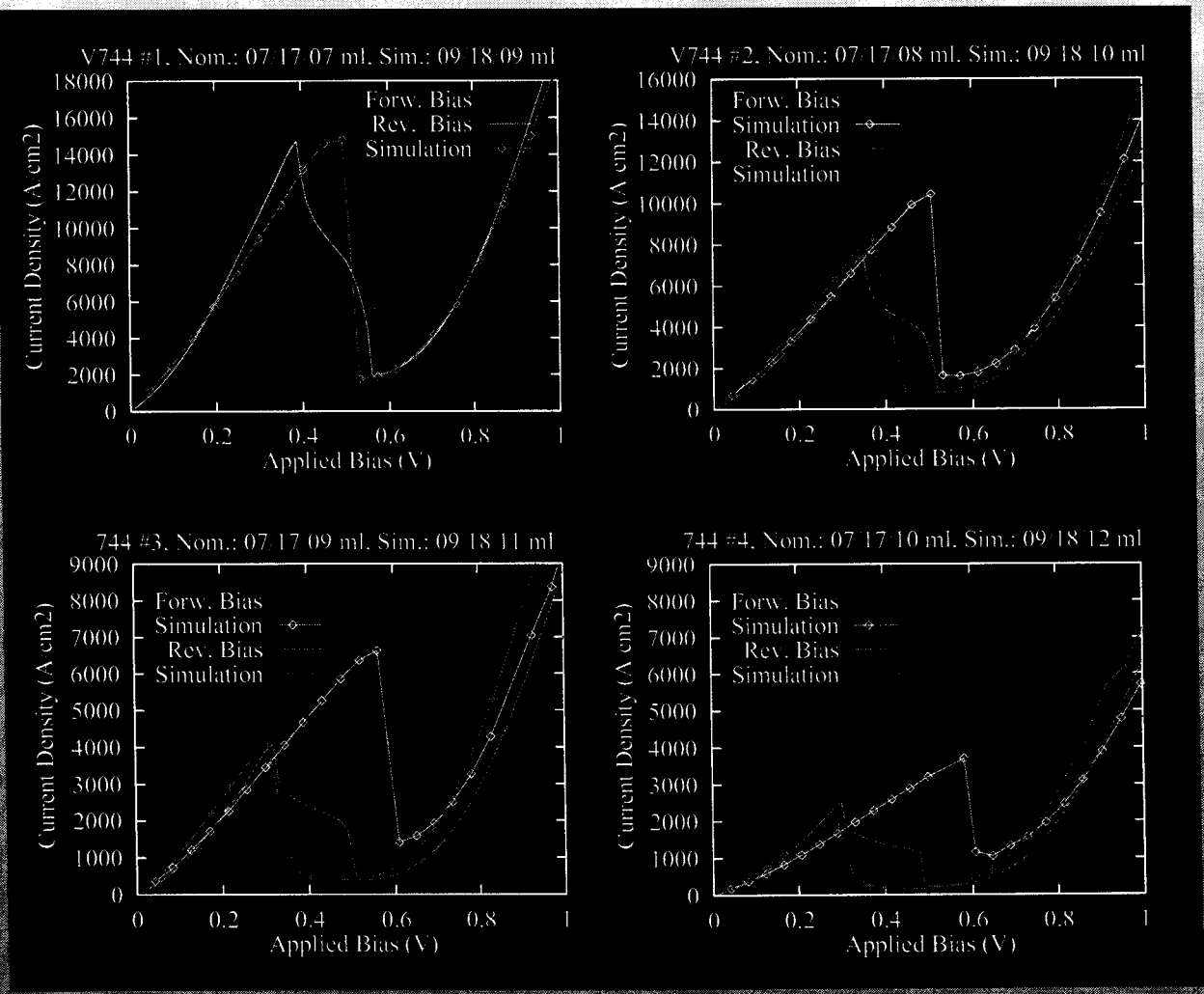
NanoElectronic MOdeling (NEMO) Simulation

Strained InGaAs/AlAs 4 Stack RTD with Asymmetric Barrier Variation

Vary One Barrier Thickness



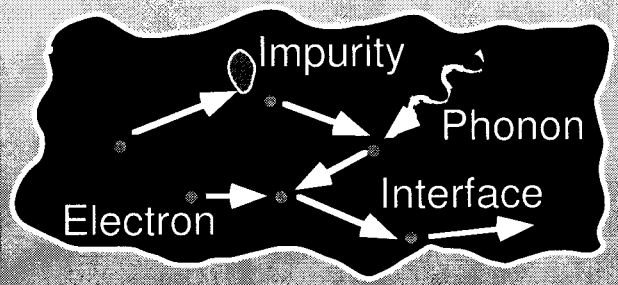
Four increasingly asymmetric devices:
20/50/20 Angstrom
20/50/23 Angstrom
20/50/25 Angstrom
20/50/27 Angstrom



Presented at IEEE DRC 1997, work performed at Texas Instrument, Dallas

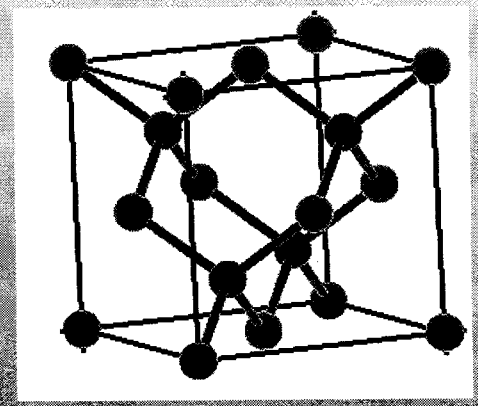
Where is NEMO compared to other models?

What is Needed for Quantum Electron Transport?



NEMO

Charging
Bandstructure
Scattering
Interference



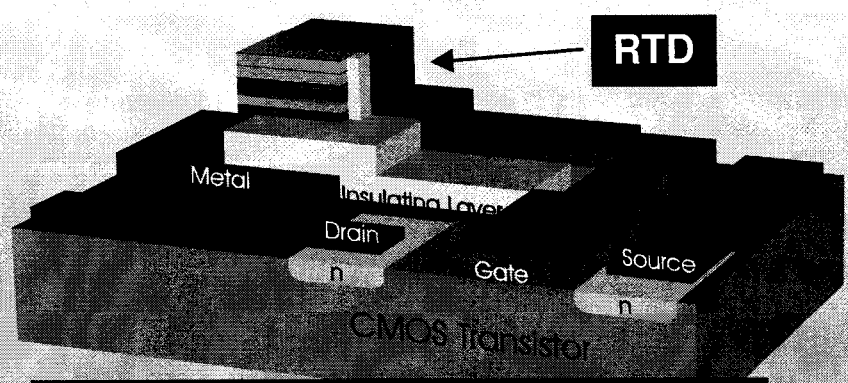
Drift-Diffusion Boltzmann Eq.

Non-Equilibrium Green Functions

Schrödinger Equation

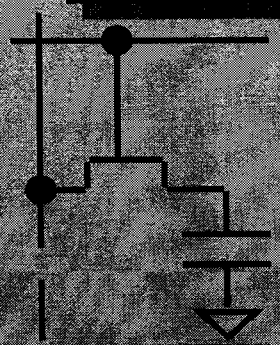
Transport with particle interaction ⟷ Quantum Mechanics

Raytheon TI Systems: Low Power RTD-based SRAM Project



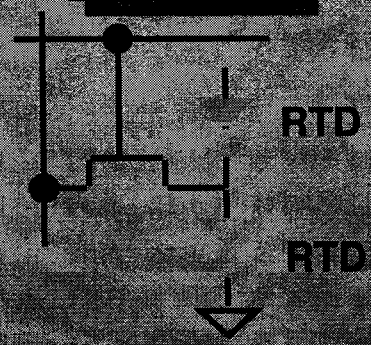
Integration of III-V RTDs with CMOS (Epitaxial Liftoff of RTD onto CMOS)

Silicon DRAM



REFRESH CIRCUITS

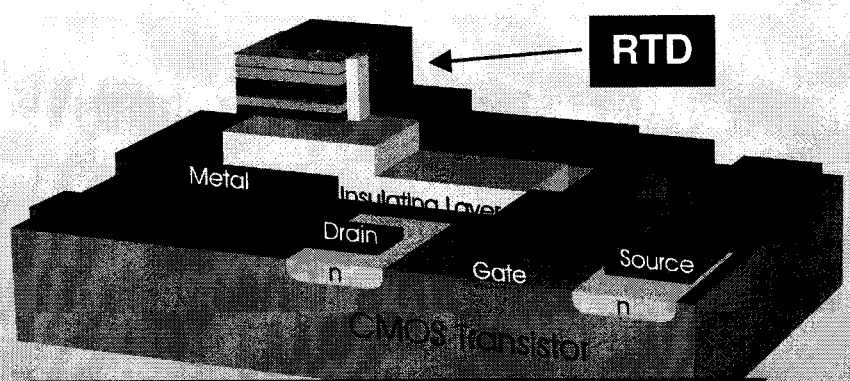
Si-QRAM



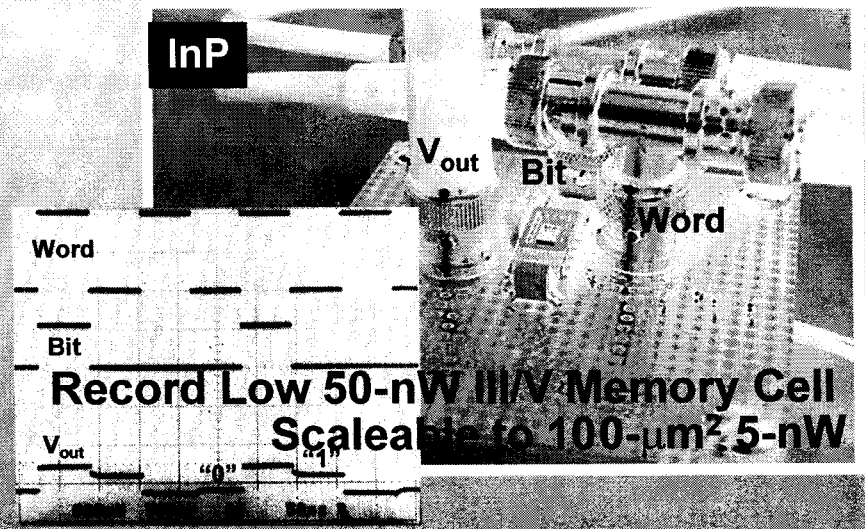
Faster, Static, & 100X Lower SBP

CONVENTIONAL → QUANTUM

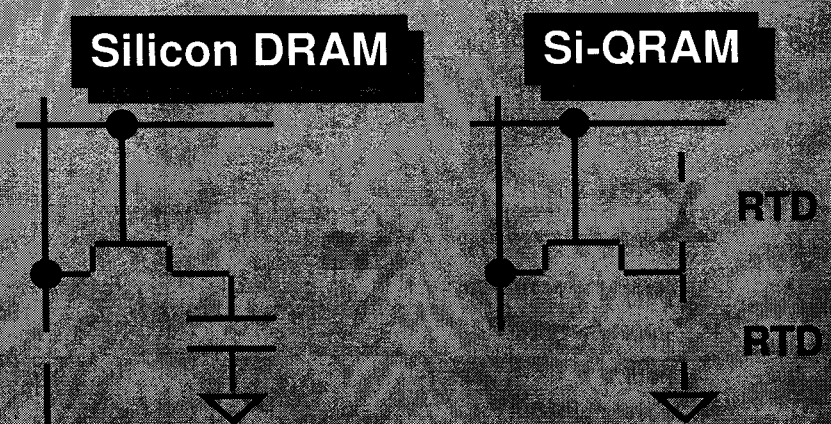
Raytheon TI Systems: Low Power RTD-based SRAM Project



Integration of III-V RTDs with CMOS
(Epitaxial Liftoff of RTD onto CMOS)



Record Low 50-nW III/V Memory Cell
Scaleable to 100-μm^2 5-nW



CONVENTIONAL → QUANTUM!

1996
- Demonstrated 100X lower power than standard GaAs SRAM
- Transferred optimized InGaAs RTDs to Georgia Tech for CMOS integration

1997
- Develop 64 kBit, 1 GHz InGaAs TSRAM (100X Density increase)
- Demonstrate RTD/CMOS memory, optical receiver, and logic.

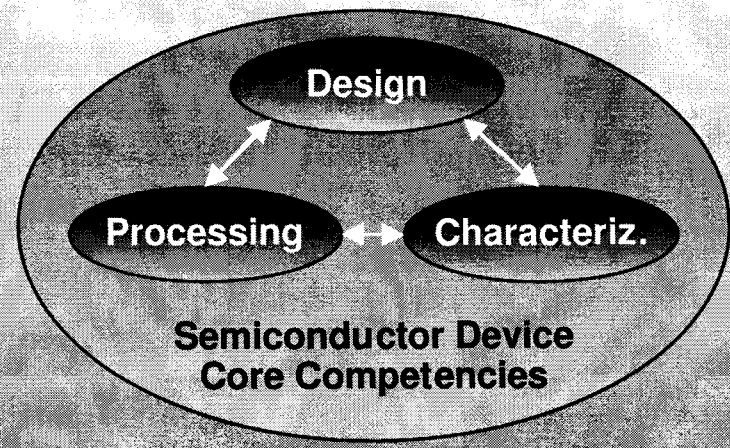
How do you know what you built?

NEMO 1-D used as Device Characterization Tool

Design:
- Circuit and device simulation is a standard tool in industry.
- Only one quantum device design tool: NEMO.

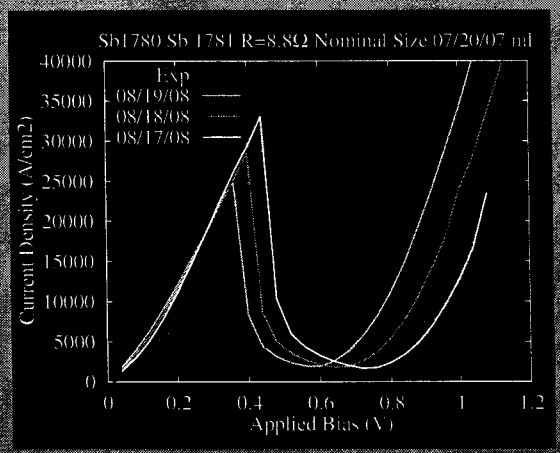
Characterization:
- **Few non-destructive tools are available on the nanometer scale.**
- **Modeling starts to show impact!**

Processing:
- Models are in their infancy.



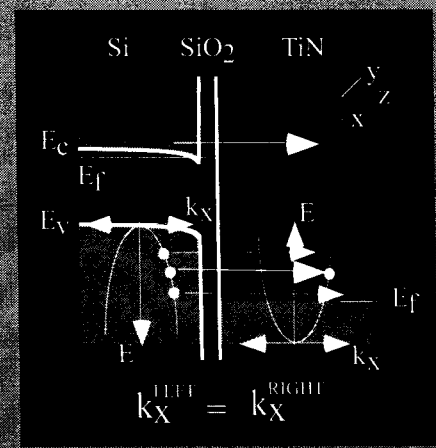
Design, Processing and Characterization are Inseparable

NEMO 1-D Usage (Raytheon/TI/JPL)



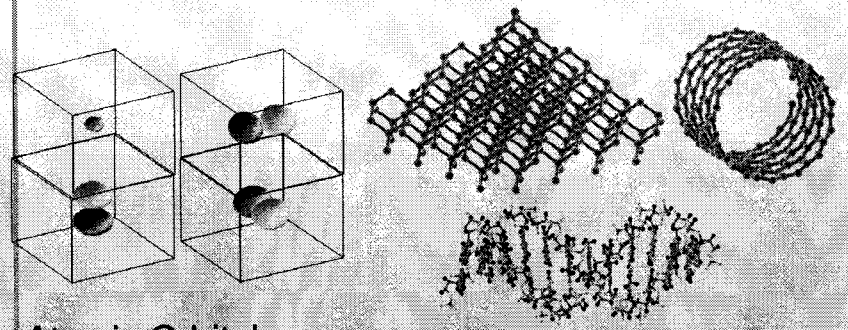
- Monolayer Sensitivity -> characteriz.
- **Genetic Algorithm SYNTHESIS / ANALYSIS**

NEMO 1-D CMOS Characterization (TI)



- Standard: Oxide thickness from capacitance.
- Thin SiO_2 (2nm) is leaky.
- $G > \omega C$
- **New:** oxide thickness from tunneling sim.

Mapping of Orbitals to Bulk Bandstructure



Atomic Orbitals
size: 0.2nm

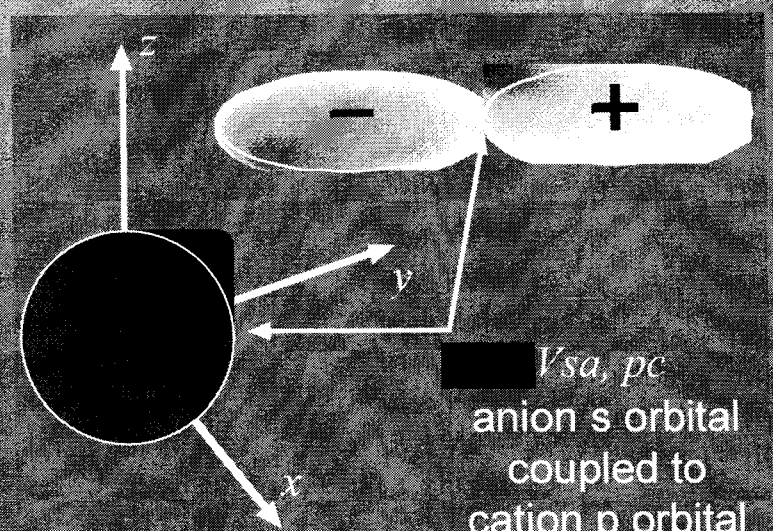
+ Structure

Bulk Semiconductors are described by:

- Conduction and valence bands, bandgaps (direct, indirect), effective masses
- 10-30 physically measurable quantities

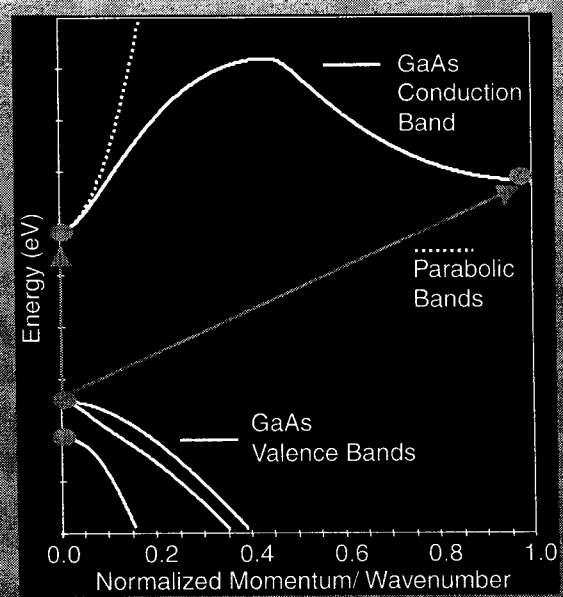
Tight Binding Models are described by:

- Orbital interaction energies.
- 15-30 theoretical parameters



Vsa, pc
anion s orbital
coupled to
cation p orbital

High
Dimensional
Fitting
Problem



15-30 theoretical interaction energies

10-30 data points of bands and masses

Global Optimization using Genetic Algorithms

Utilizing Evolutionary Principles of Survival of the Fittest

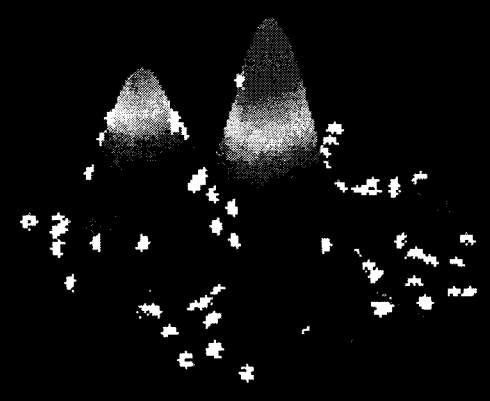
Genetic Algorithm Overview:

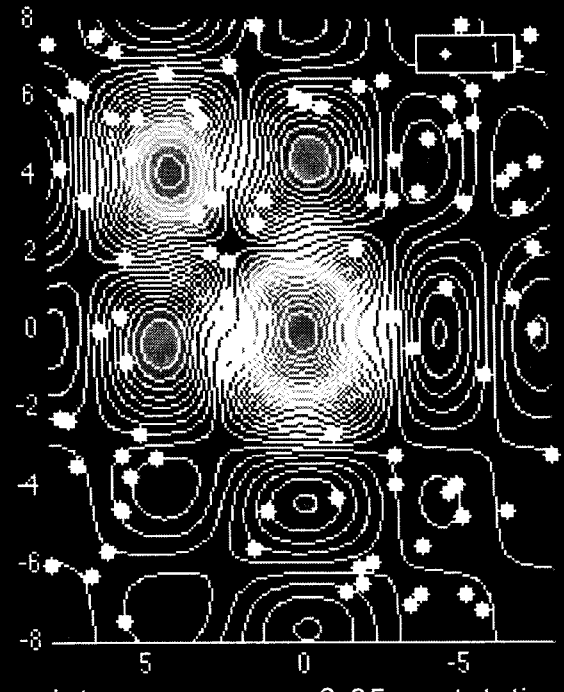
Stochastic placement of individuals in the search/design space.

Every Generation eliminate "unfit" elements and create new ones from survivors.

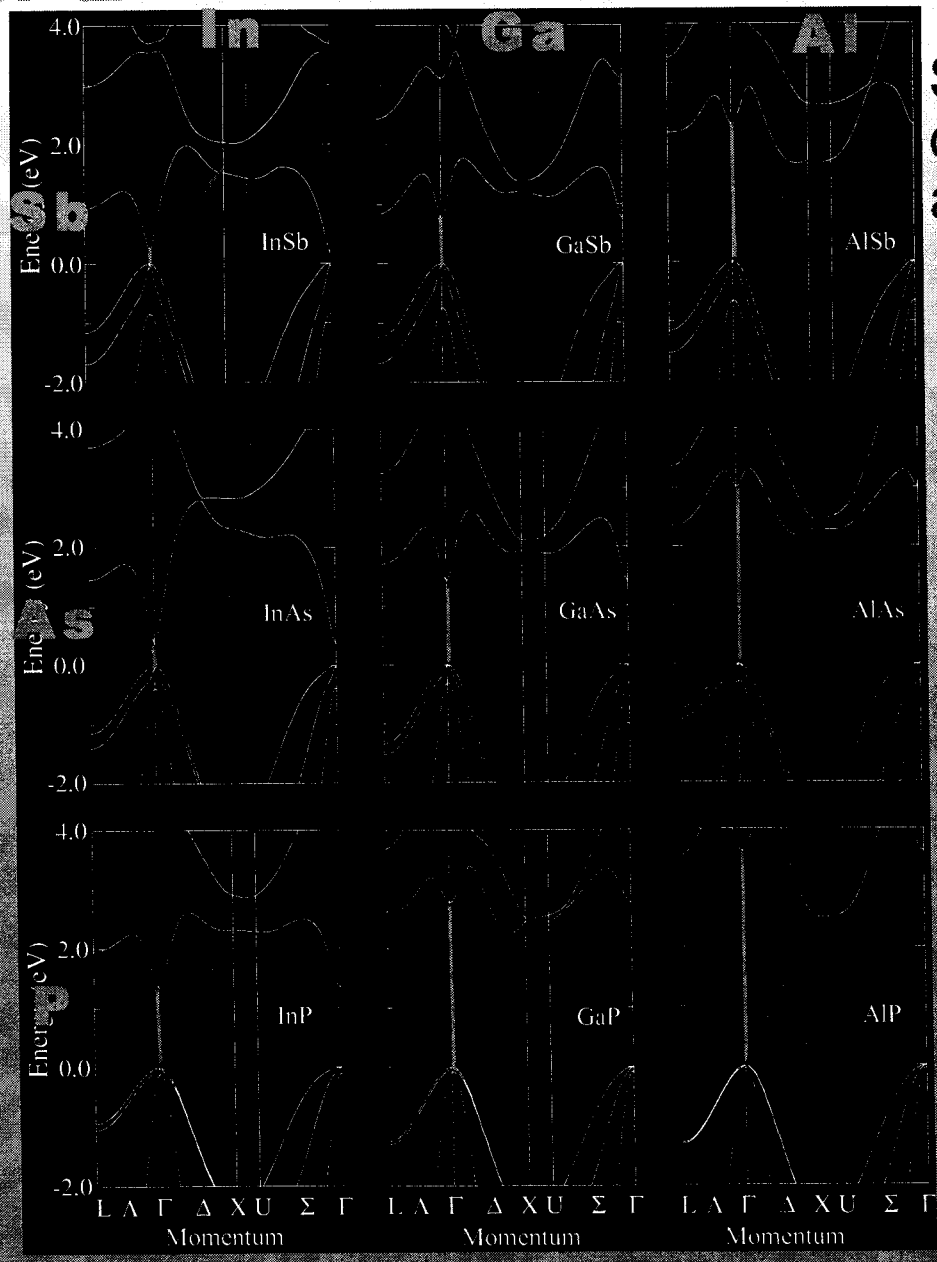
Reevaluate the fitness of population.

$$F(x,y) = \frac{\sin(x)}{x}\frac{\sin(y)}{y} + 0.7\,\frac{\sin(x-4)}{(x-4)}\frac{\sin(y-4)}{(y-4)}$$



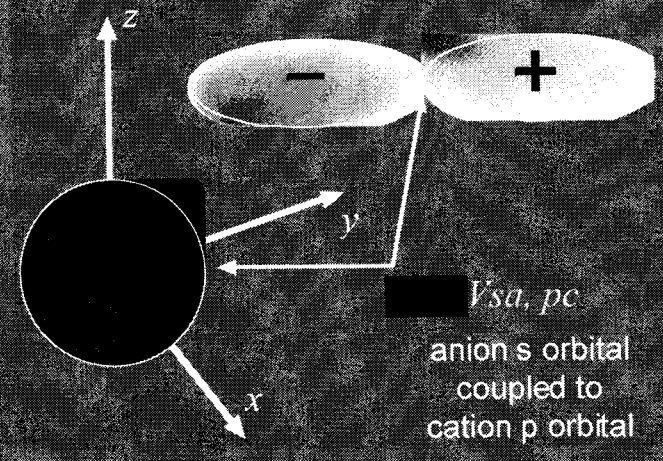


pop = 100, 300 generations, steady-state (10%), 2-point crossover p = 0.85, mutatation p = 1/2



Semiconductor Compounds:
cation: In, Ga, Al
anion: Sb, As, P

- Match experimental data in various electron transport areas of the Brillouin zone:
  - Effective masses of electrons at Γ, X and L
  - Effective masses of holes at Γ
  - Bandedges at Γ, X and L
- Each individual material poses a 15 dimensional fitting problem.



Genetically Engineered Nanoelectronic Structures (GENES)

Objectives:

- Automate nanoelectronic device synthesis, analysis, and optimization using genetic algorithms (GA).

NASA Relevance:

- Generation of novel devices for in-situ measurements of spectral lines.
- Contribution to revolutionary computing efforts using quantum dots.

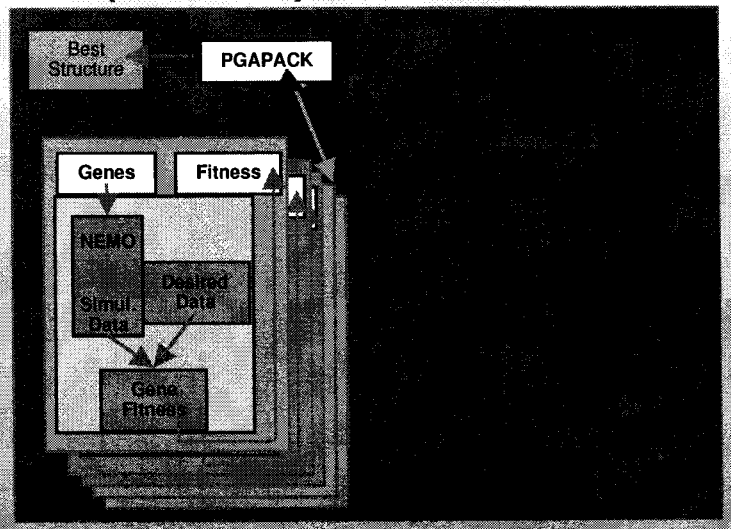
Approach:

- Augment parallel genetic algorithm (PGApack).
- Combine PGApack with NEMO.
- Develop graphical user interface for GA.

Publications:

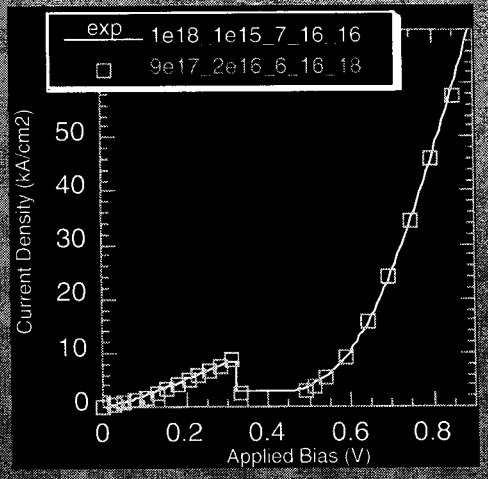
- MRS Proc. Vol. 551, 149 (1999), 2 in press Superl. Microstruct.

Architecture



Results:

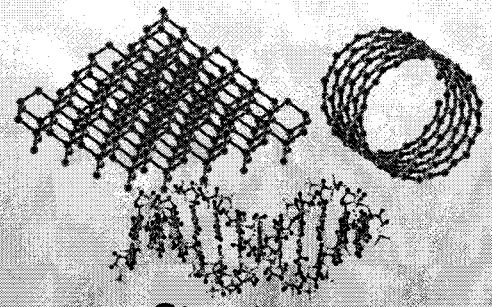
Nanoelectronic Device Structural analysis



GA analyzed atomic monolayer structure and doping profile of RTD device
Black: structure specs, Blue: Best fit

Dissimilar Compounds Experience Strain!

Strain Modifies Electronic Characteristics!



Structure

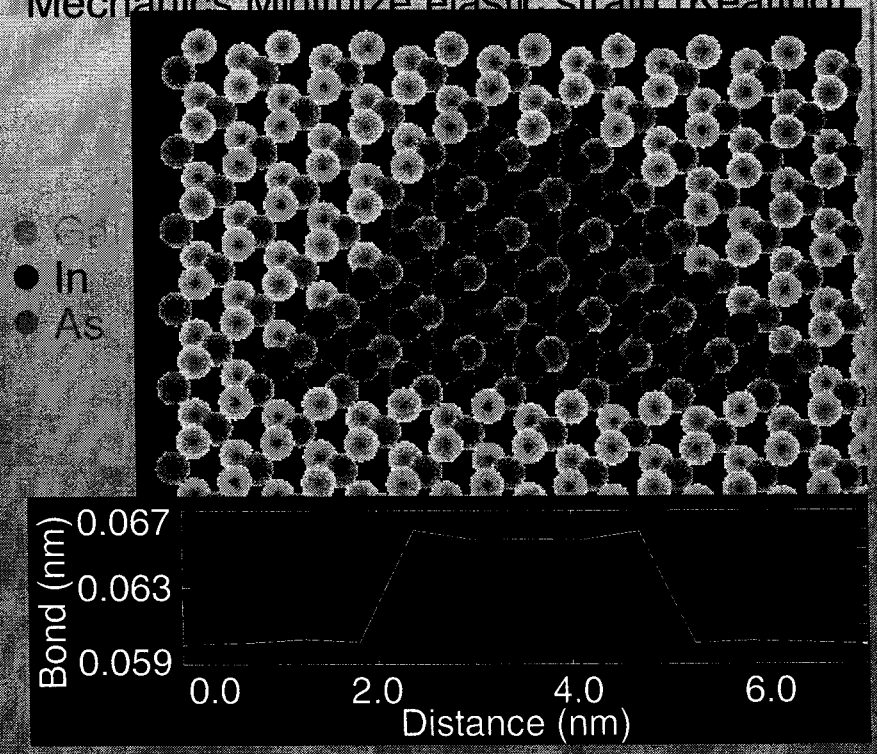
Dot Formation Due to Strain:

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

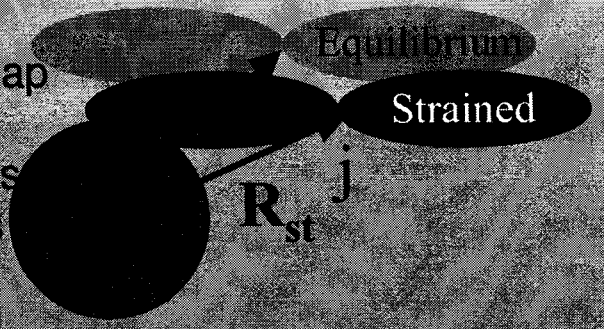
Strain affects Electronic Structure:

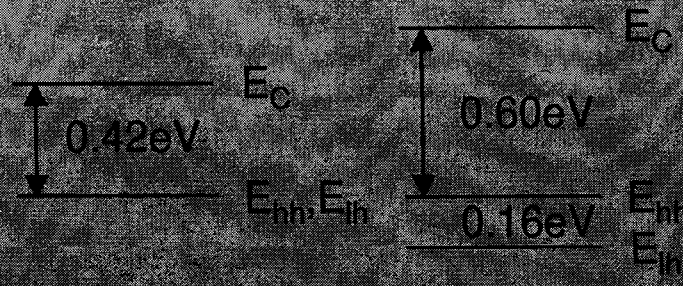
- Tight binding models can predict this!

Mechanics:Minimize elastic strain (Keating)



Electronics:
Orbital overlap changes
=> bandgaps and masses

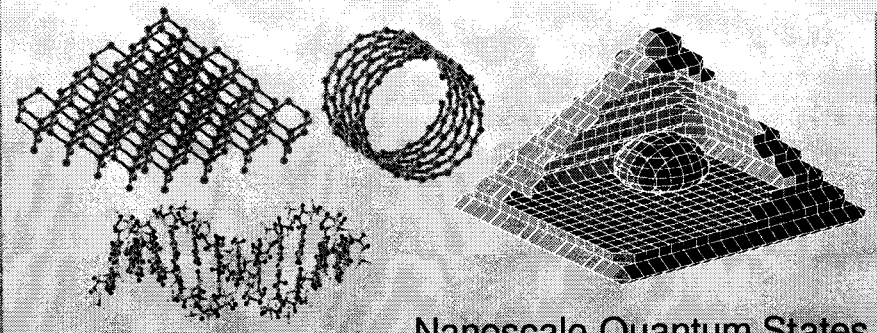




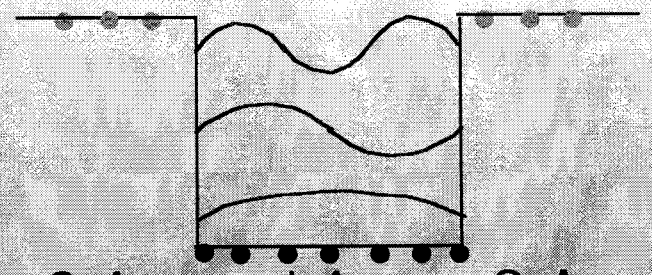
InAs at 4K in GaAs/InAs/GaAs superlattice.
Brühbach et al. Superlatt.&Microstr. V21, n.4 (1997)

Dissimilar Materials Create Quantum Confinement

Nanoscale Quantum States Emerge



Structure → Nanoscale Quantum States (Artificial Atoms, size 20nm)



Objective:

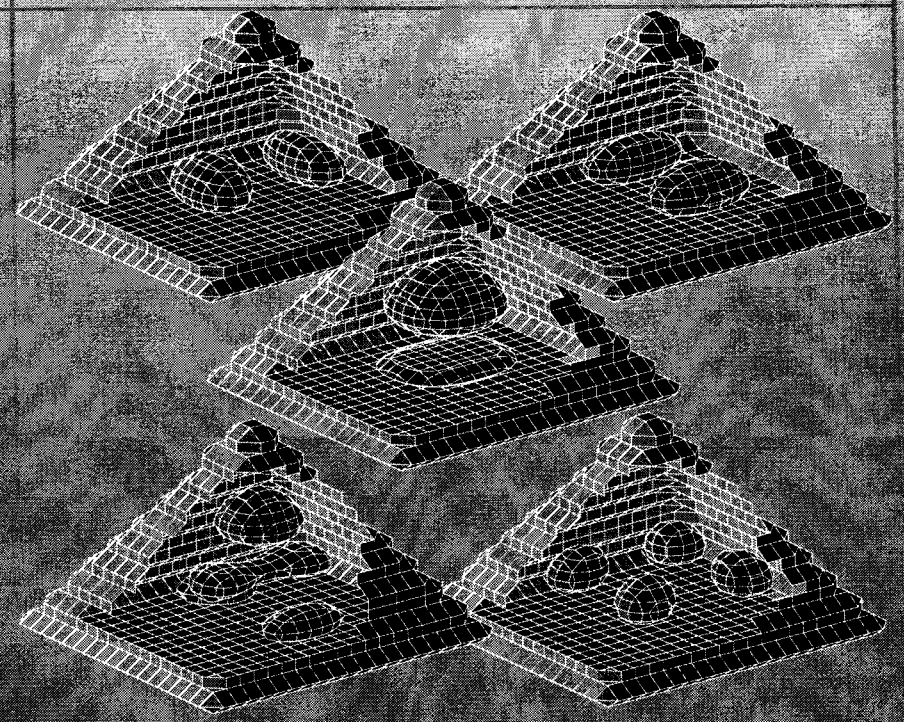
- Need to locate new quantum state energies and wave functions.

Problem:

- Realistic Quantum Dots consist of about 10^6 atoms
- Realistic system is OPEN

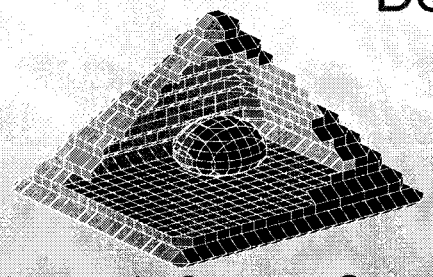
Approach:

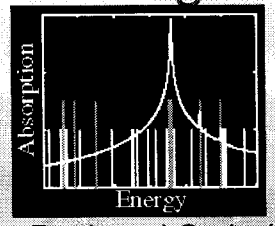
- Custom Lanczos Eigenvalue Solver for Hermitian and non-Hermitian Matrices
- Massively parallel implementation.



Quantum Dots as Optical Detectors

Desensitizing QWIP to Polarization



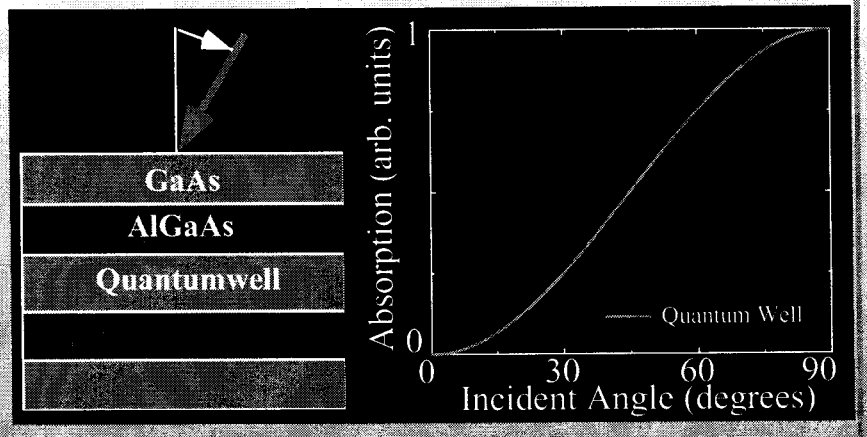


Nanoscale Quantum States
(Artificial Atoms, size 20nm)

Designed Optical Transitions

Sensors

- Problem: Quantum wells are "blind" to light impinging orthogonal to the detector.
- Standard Solution:grating turns polarization
- New Approach: Quantum dots have a built-in anisotropy -> absorption at all angles

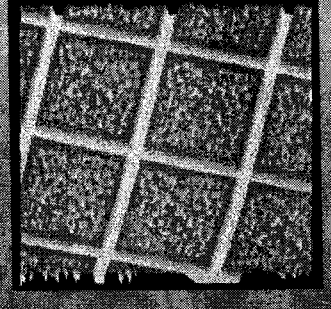


Quantum Wells: Absorption has strong incidence angle dependence

Electromagnetic Modeling

Standard Solution:

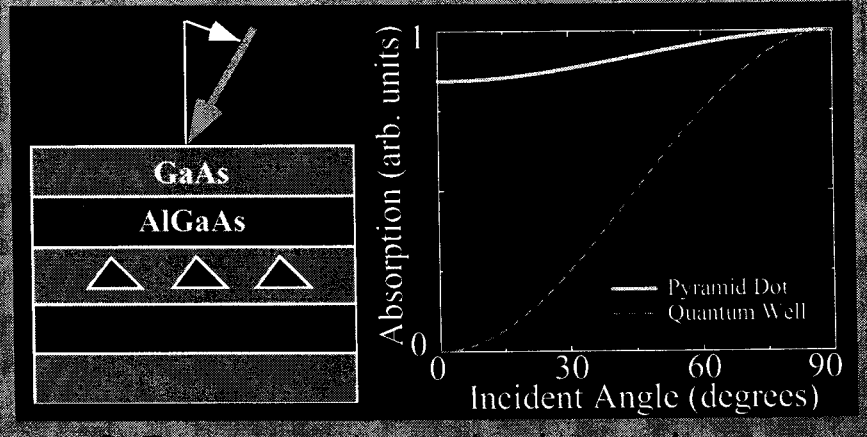
Grating



electric field models

↓

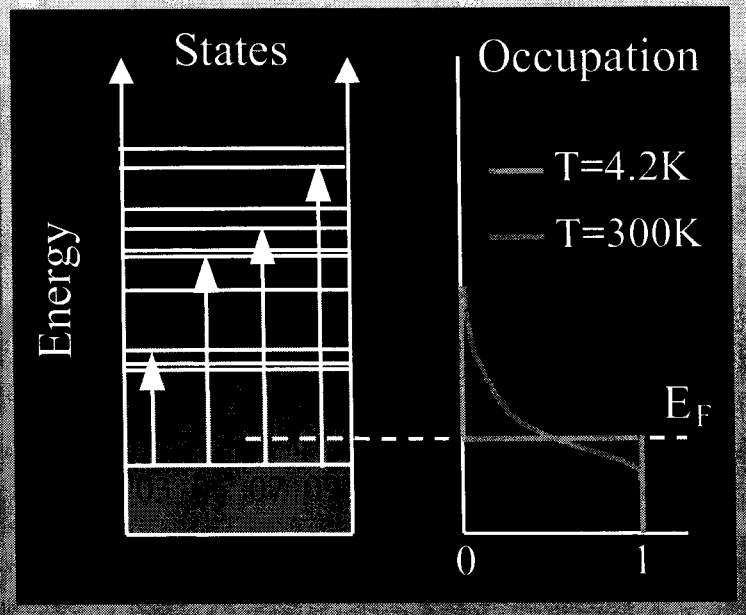
optimized light coupling



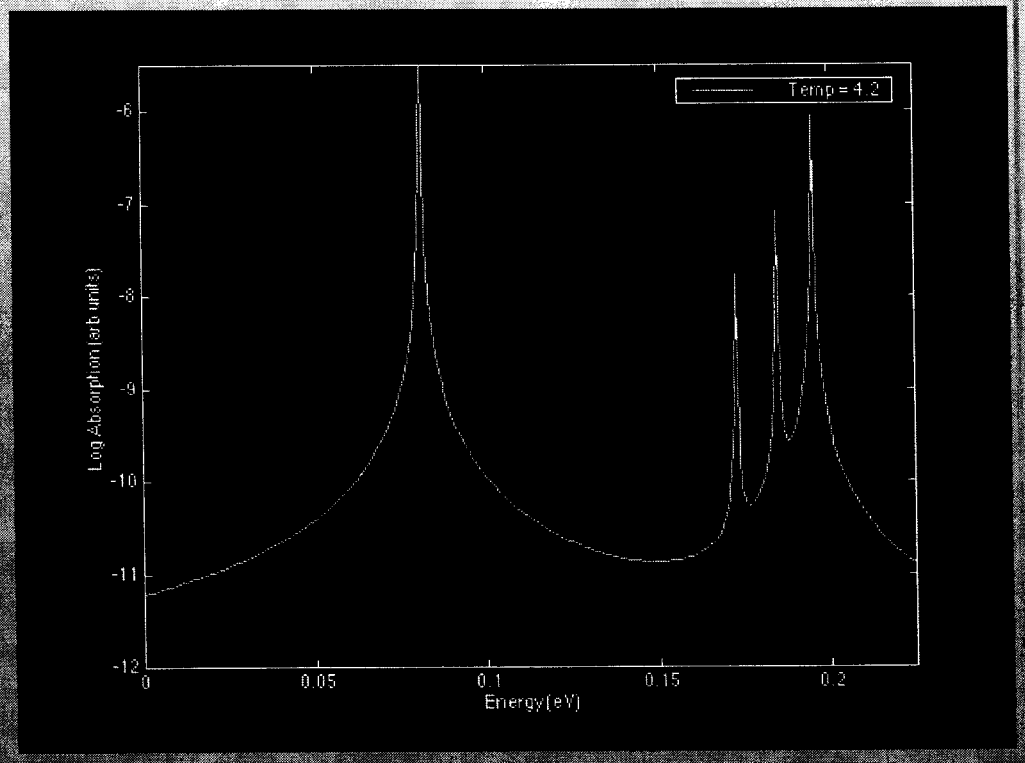
Q Dots: weak angle dependence
Radiation Hard

Temperature Dependence of Quantum Dot Absorption Spectrum

State Occupation



Absorption



Higher temperatures

↓

More occupied states

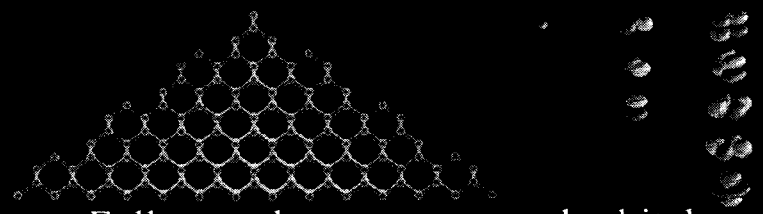
↓

More transitions.

Accomplishments & Plans

1999 Accomplishments

Atomistic Tight-Binding Hamiltonian



Full crystal symmetry; s,p,d orbitals

Atomistic Strain Model

Atomic locations Scale bond interactions

Parallel Lanczos Eigensolver

FLOPS scale $N^{1.1}$ => 10^6 Atoms!

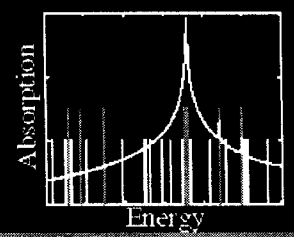
Genetic Algoritms: Optimized Basis Sets and Nanostructure device analysis

GUI: Client Server Tcl/Tk, SQL Database

Optical Interactions

Electric Dipole Transitions

Absorption vs. Energy



2000/2001 Plans

Physics

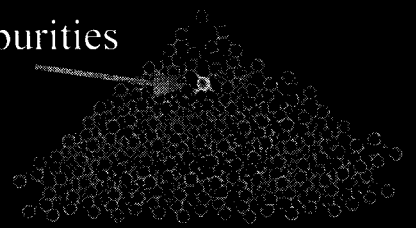
- Hatree-Fock potential
- Piezo-electric effects
- Many-body via configuration interaction
- Rate equation based transport

Software

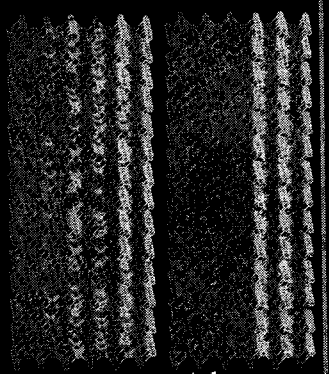
- Develop 3D visualization
- Shared-memory parallelization (OpenMP)

Quantum Dot Simulations

Impurities

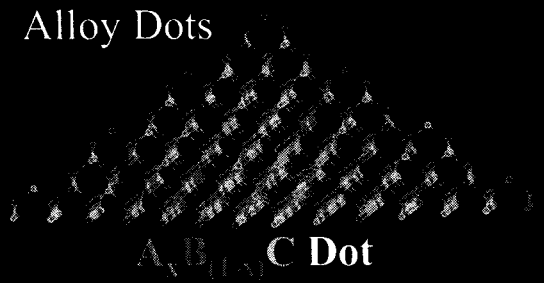


Grading



Graded Abrupt

Alloy Dots



$A_xB_{(1-x)}C$ Dot

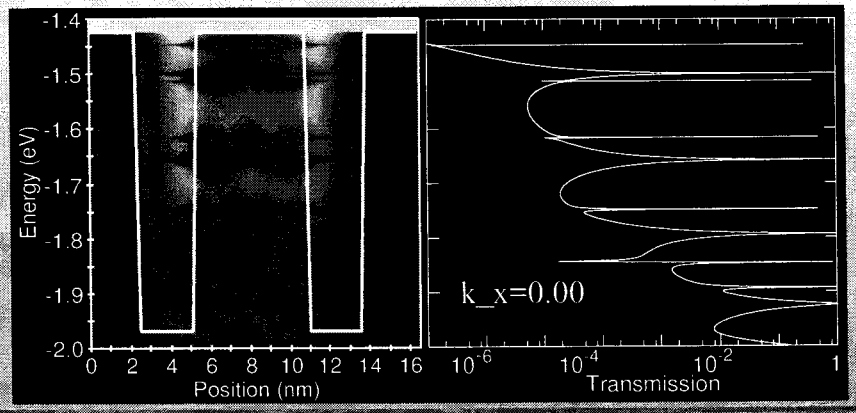
No Time to Talk About:

Hole Transport in Heterostructures:
- **Resonant Tunneling Diodes**
- **Cascade Lasers**

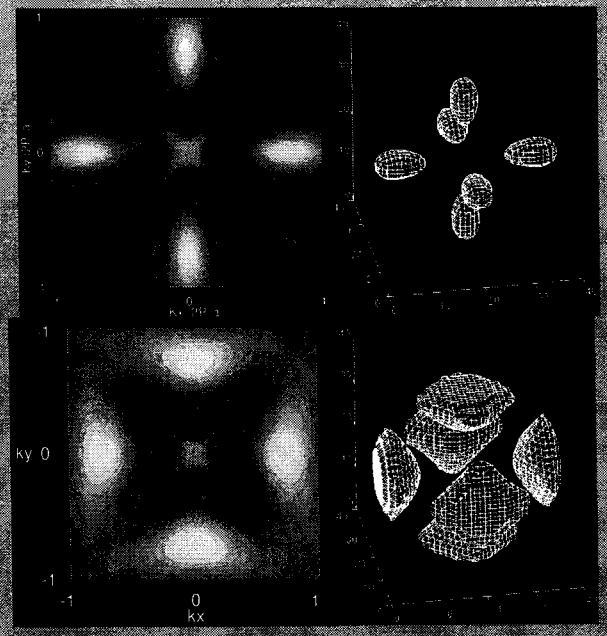
THz response in Heterostructures:
- **Resonant Tunneling Diode**

Limitations of Bandstructure Models.

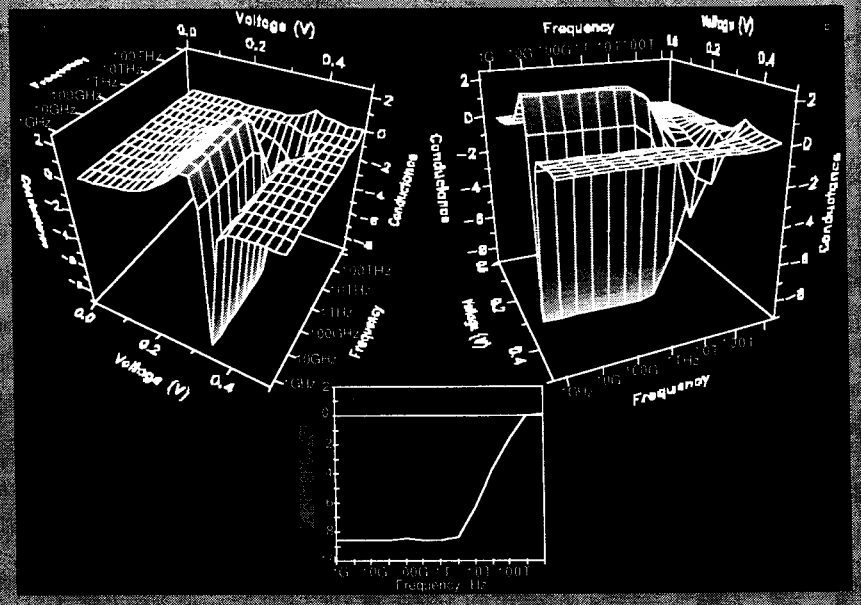
Hole Transport



Bandstructure Model Limitations



THz Response of a RTD



State of the Art:
Only we are set-up to do Molectronics!

Investigator	Location	Hamiltonian	Atomistic	Many-Body	Extendable to Molecules?
Pryor	Lund	k•p	NO	YES	NO
Bimberg	Berlin	k•p	NO	NO	NO
Freund	Brown	k•p	NO	NO	NO
Leburton	Illinois	1 Band	NO	NO	NO
Zunger	NREL	Pseudopotential	YES	NO	NO
Bowen Klimeck	JPL	Tight-binding	YES	NO*	YES

* - Planned for 00/01

Carbon Nanotubes

Nanospace 2000 Discussions:

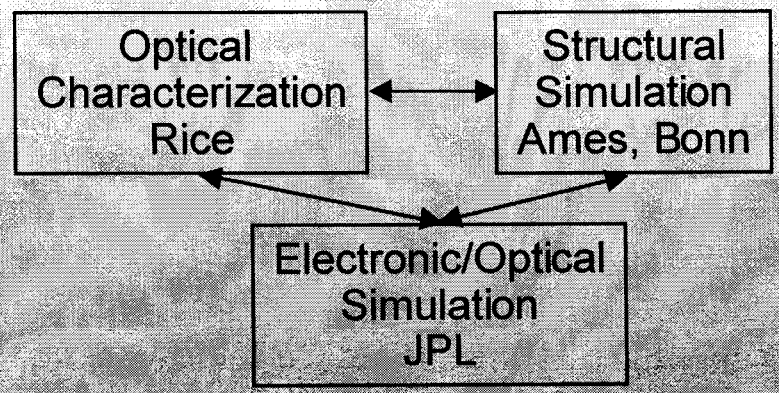
Bob Hauge (Rice U.):

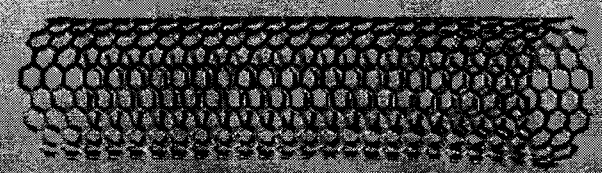
- If you have a general 3D modeling tool, can you model Nanotubes?
- We need theoretical optical absorption simulations to establish a fingerprint database for the tubes that are in the solution.

Deepak Srinivastava (Ames), Attila Caglar (Bonn):

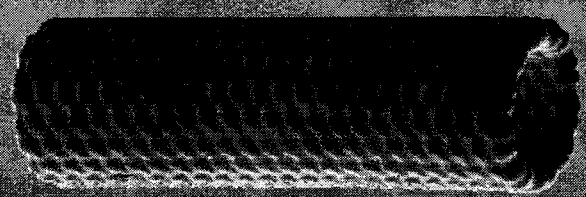
- We can give you nanotube structures (from molecular dynamics simulation)

Possible Cooperation:

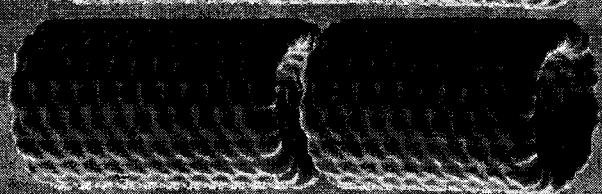




Nanotube

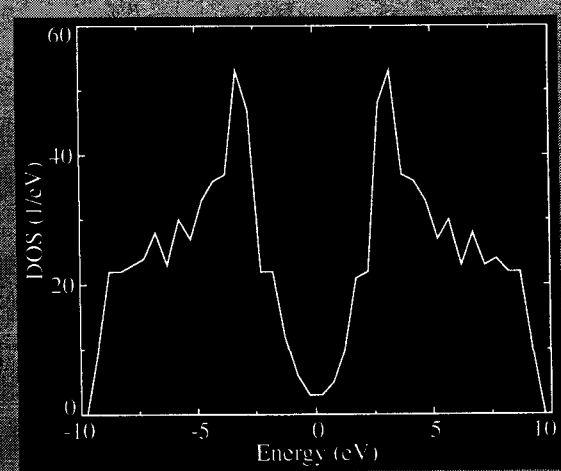


Ground State



1st excited State

Density of States



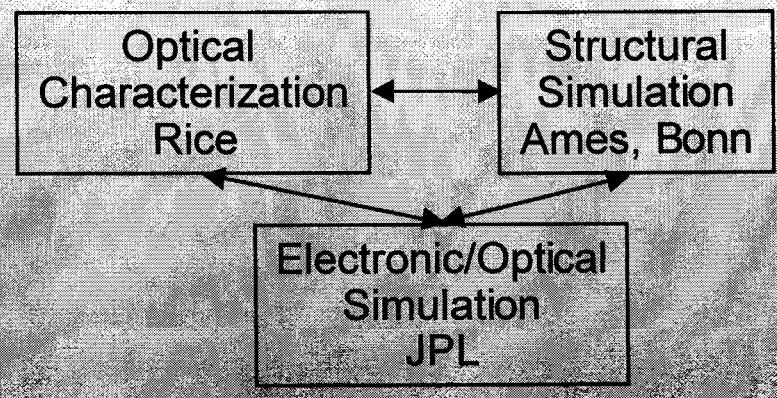
Carbon Nanotubes Simulations at JPL?

Optical Simulations

- Establish a fingerprint map of the absorption of "all" ideal nanotubes.

-> help decipher experimental data that probes optically MANY different nanotubes in the production process

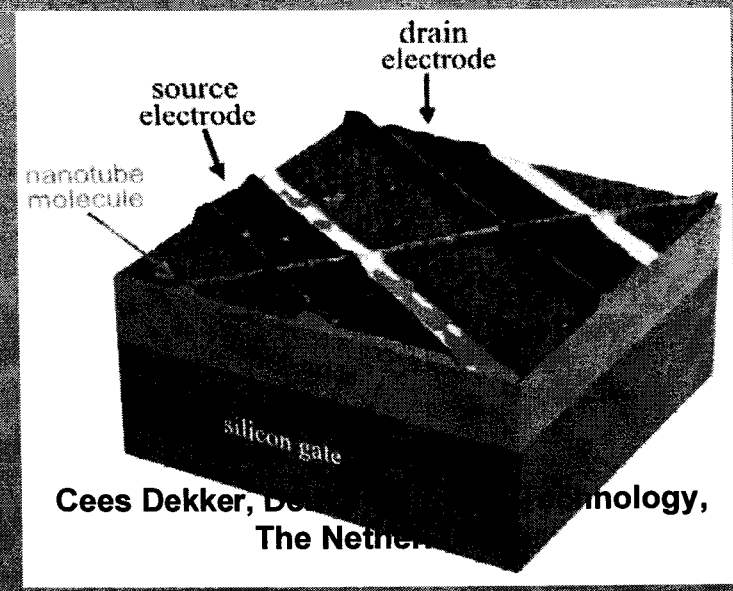
Possible Cooperation:



Electron transport

- Charge transport in non-ideal tubes:
  - bent, stretched, layered over contacts
  - charge injection from the side of the tubes, instead of the end
  - -> what is the REAL resistance of the tubes?

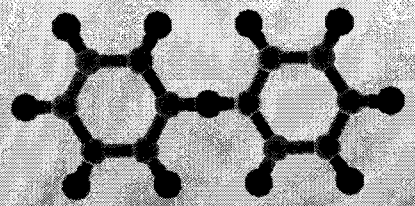
Nanotube FET

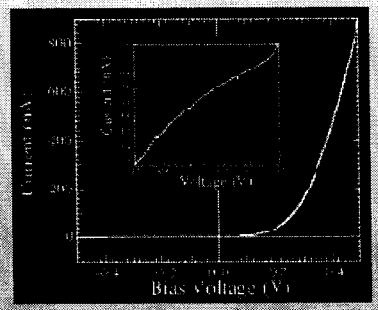


Cees Dekker, De... ...nology, The Nether...

Molectronics

Molecular Electronics



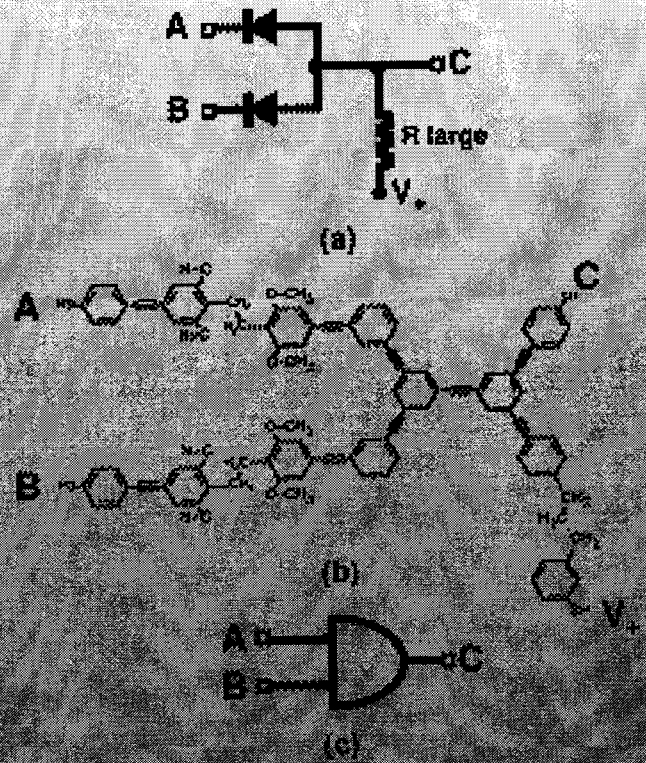


Polyphenylene "Diode"

Molecular Biosensors

DNA based in-vivo sensor

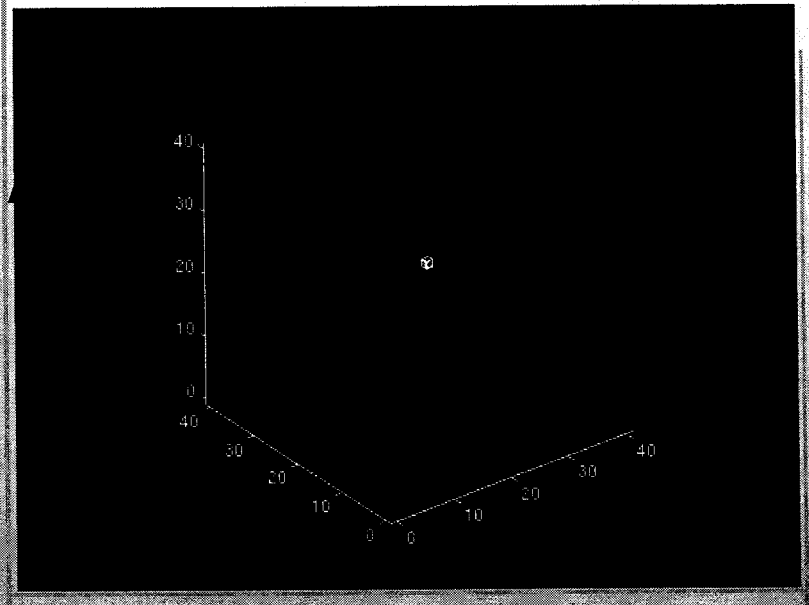
Molectronic AND Gate



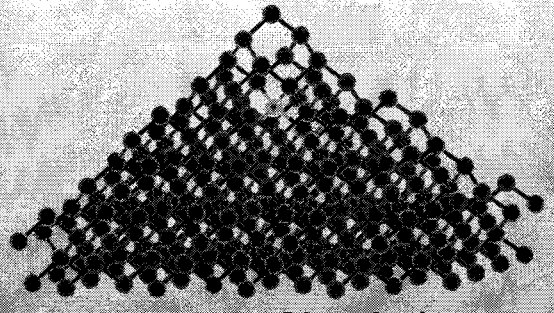
A	B	C
0	0	0
1	0	0
0	1	0
1	1	1

(d)

Future Vision

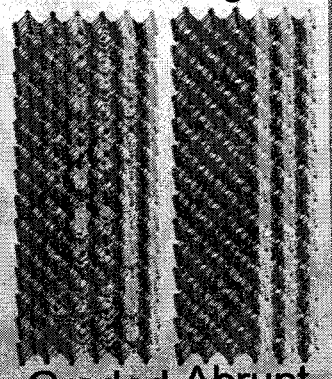


Quantum Dots



Atomistic Simulation

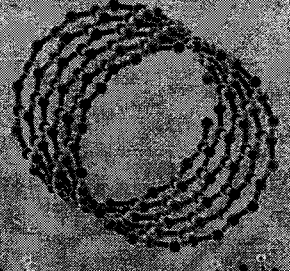
Grading



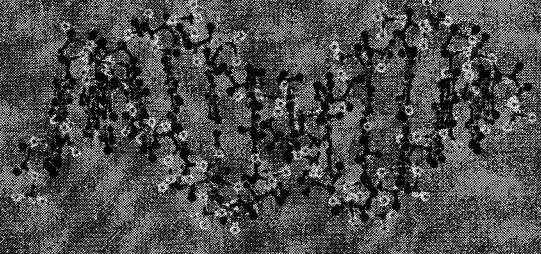
Graded Abrupt

Transport in Molecules

Carbon Nanotubes



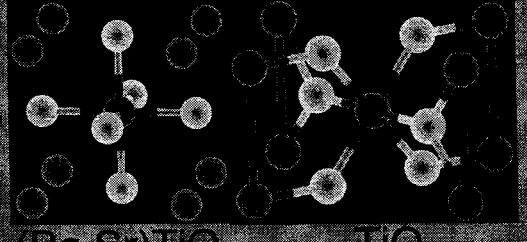
DNA



End of SIA Roadmap

Dopant Fluctuations in Ultra-scaled CMOS

Electron Transport in Exotic Dielectrics



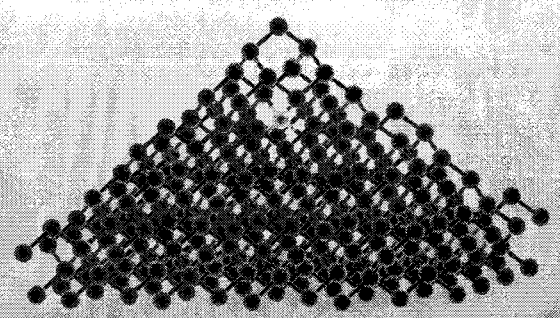
$(Ba,Sr)TiO_3$ TiO_2

Future Vision

Atomistic Simulation Tool

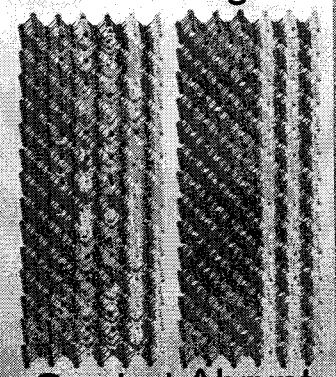
- General Structure Input
- Address CMOS Scaling Issues.
- Orbital Basis Extends to Molecules

Quantum Dots



Atomistic Simulation

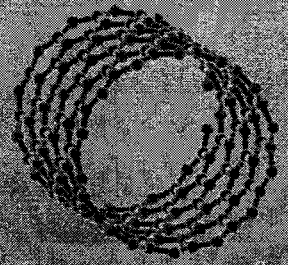
Grading



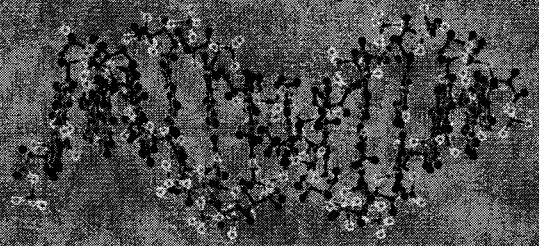
Graded Abrupt

Transport in Molecules

Carbon Nanotubes

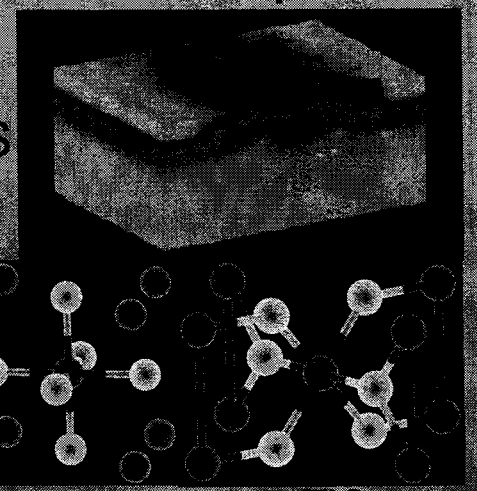


DNA



End of SIA Roadmap

Dopant Fluctuations in Ultra-scaled CMOS



Electron Transport in Exotic Dielectrics

$(Ba,Sr)TiO_3$ TiO_2